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

Plan for Lecture 20:

Review Chapters 1-4,6,7

1. Scattering theory & Rotation reference frames
2. Calculus of variation
3. Lagrangian and Hamiltonian formalisms
4. Normal modes of vibration
5. The wave equation
6. Sturm-Liouville equation

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	Date	F&W Reading	Topic	Assignment	Due
1	Mon, 8/26/2019	Chap. 1	Introduction	#1	8/30/2019
2	Wed, 8/28/2019	Chap. 1	Scattering theory	#2	9/02/2019
3	Fri, 8/30/2019	Chap. 1	Scattering theory	#3	9/04/2019
4	Mon, 9/02/2019	Chap. 1	Scattering theory	#4	9/06/2019
5	Wed, 9/04/2019	Chap. 2	Non-inertial coordinate systems	#5	9/09/2019
6	Fri, 9/06/2019	Chap. 3	Calculus of Variation	#6	9/11/2019
7	Mon, 9/9/2019	Chap. 3	Calculus of Variation	#7	9/13/2019
8	Wed, 9/11/2019	Chap. 3	Lagrangian Mechanics		
9	Fri, 9/13/2019	Chap. 3	Lagrangian Mechanics	#8	9/16/2019
10	Mon, 9/16/2019	Chap. 3 & 6	Constants of the motion	#9	9/20/2019
11	Wed, 9/18/2019	Chap. 3 & 6	Hamiltonian equations of motion		
12	Fri, 9/20/2019	Chap. 3 & 6	Liouville theorm	#10	9/23/2019
13	Mon, 9/23/2019	Chap. 3 & 6	Canonical transformations		
14	Wed, 9/25/2019	Chap. 4	Small oscillations about equilibrium	#11	9/30/2019
15	Fri, 9/27/2019	Chap. 4	Normal modes of vibration	#12	10/02/2019
16	Mon, 9/30/2019	Chap. 7	Motion of strings	#13	10/04/2019
17	Wed, 10/02/2019	Chap. 7	Sturm-Liouville equations	#14	10/07/2019
18	Fri, 10/04/2019	Chap. 7	Sturm-Liouville equations		
19	Mon, 10/07/2019	Chap. 7	Fourier transform methods		
20	Wed, 10/09/2019	Chap. 1-4,6-7	Review		
	Fri, 10/11/2019	No class	Fall break		
	Mon, 10/14/2019	No class	Take-home exam		
	Wed, 10/16/2019	No class	Take-home exam		
21	Fri, 10/18/2019	Chap. 7	Take-home exam due		

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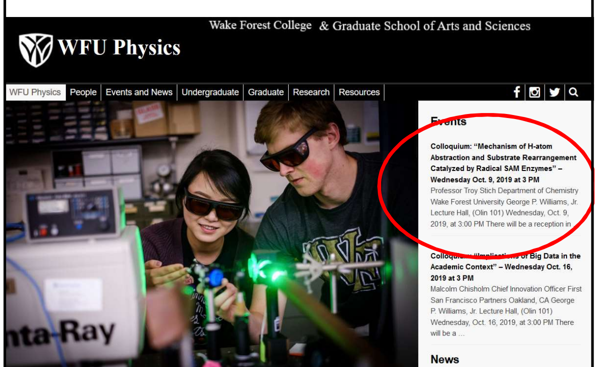

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Troy Stich, PhD

Department of Chemistry
Wake Forest University
3 PM Olin 101
"Mechanism of H-atom Abstraction and Substrate Rearrangement Catalyzed by Radical SAM Enzymes"

The radical SAM (S-adenosyl-L-methionine) superfamily of enzymes catalyzes a dizzying array of chemistries triggered by reductive cleavage of SAM to yield the primary carbon radical 5'-deoxyadenosyl (5'dAdo•). 5'dAdo• can pluck off H-atoms with bond dissociation enthalpies <105 kcal/mol from substrate molecules to initiate carbon skeleton rearrangements. We hypothesize that amino acids within the active site, a triose phosphate isomerase (TIM) barrel, are key in conducting these rearrangements down the evolutionary-designed path. Our research effort employs a combined biochemical, spectroscopic, and computational approach to determine atomic level details of these mechanisms. We further use substrate analogs that can slow or halt the chemistry at key points, allowing

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Scattering theory

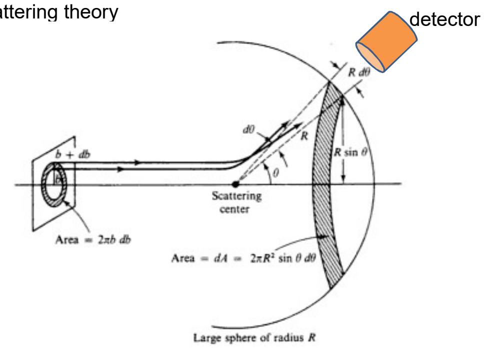

Figure 5.5 The scattering problem and relation of cross section to impact parameter.

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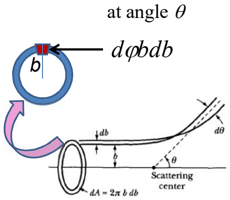
Differential cross section

$$\left(\frac{d\sigma}{d\Omega}\right) = \frac{\text{Number of detected particles at } \theta \text{ per target particle}}{\text{Number of incident particles per unit area}}$$

= Area of incident beam that is scattered into detector at angle θ



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

Figure from Marion & Thorton, Classical Dynamics

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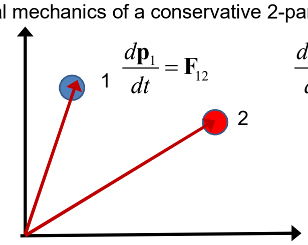
Relationship of scattering cross-section to particle interactions -- Classical mechanics of a conservative 2-particle system.



$$\frac{d\mathbf{p}_1}{dt} = \mathbf{F}_{12} \qquad \frac{d\mathbf{p}_2}{dt} = \mathbf{F}_{21}$$

$$\mathbf{F}_{12} = -\nabla_1 V(\mathbf{r}_1 - \mathbf{r}_2) \quad \Rightarrow E = \frac{1}{2}m_1 v_1^2 + \frac{1}{2}m_2 v_2^2 + V(\mathbf{r}_1 - \mathbf{r}_2)$$

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Relationship between center of mass and laboratory frames of reference

Definition of center of mass $\mathbf{R}_{CM}$

$$m_1\mathbf{r}_1 + m_2\mathbf{r}_2 = (m_1 + m_2)\mathbf{R}_{CM}$$

$$m_1\dot{\mathbf{r}}_1 + m_2\dot{\mathbf{r}}_2 = (m_1 + m_2)\dot{\mathbf{R}}_{CM} = (m_1 + m_2)\mathbf{V}_{CM}$$

$$E = \frac{1}{2}m_1 v_1^2 + \frac{1}{2}m_2 v_2^2 + V(\mathbf{r}_1 - \mathbf{r}_2)$$

$$= \frac{1}{2}(m_1 + m_2)V_{CM}^2 + \frac{1}{2}\mu|\mathbf{v}_1 - \mathbf{v}_2|^2 + V(\mathbf{r}_1 - \mathbf{r}_2)$$

where: $\mu \equiv \frac{m_1 m_2}{m_1 + m_2}$

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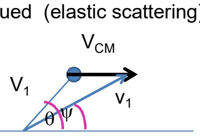
Relationship between center of mass and laboratory frames of reference – continued (elastic scattering)



$$\mathbf{v}_1 = \mathbf{V}_1 + \mathbf{V}_{CM}$$

$$v_1 \sin\psi = V_1 \sin\theta$$

$$v_1 \cos\psi = V_1 \cos\theta + V_{CM}$$

$$\tan\psi = \frac{\sin\theta}{\cos\theta + V_{CM}/V_1} = \frac{\sin\theta}{\cos\theta + m_1/m_2}$$

$$\text{Also:} \quad \cos\psi = \frac{\cos\theta + m_1/m_2}{\sqrt{1 + 2m_1/m_2\cos\theta + (m_1/m_2)^2}}$$

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Differential cross sections in different reference frames – continued:

$$\left(\frac{d\sigma_{LAB}(\psi)}{d\Omega_{LAB}}\right)=\left(\frac{d\sigma_{CM}(\theta)}{d\Omega_{CM}}\right)\left|\frac{d\cos\theta}{d\cos\psi}\right|$$

$$\left(\frac{d\sigma_{LAB}(\psi)}{d\Omega_{LAB}}\right)=\left(\frac{d\sigma_{CM}(\theta)}{d\Omega_{CM}}\right)\frac{\left(1+2m_1/m_2\cos\theta+(m_1/m_2)^2\right)^{3/2}}{(m_1/m_2)\cos\theta+1}$$

$$\text{where : }\quad \tan\psi=\frac{\sin\theta}{\cos\theta+m_1/m_2}$$

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Calculation of elastic scattering cross section in the center of mass frame of reference for central potential *V(r)*

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

$$\theta=-\pi+2b\int_{r_{\min}}^{\infty}dr\left(\frac{1/r^2}{\sqrt{1-\frac{b^2}{r^2}-\frac{V(r)}{E}}}\right)$$

where $r_{\min}$ is found from

$$1-\frac{b^2}{r_{\min}^2}-\frac{V(r_{\min})}{E}=0$$

Conserved energy in CM frame

Distance of closest approach

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Application of Newton's laws in a coordinate system which has an angular velocity $\boldsymbol{\omega}$ and linear acceleration $\left(\frac{d^2\mathbf{a}}{dt^2}\right)_{inertial}$

Newton's laws; Let $\mathbf{r}$ denote the position of particle of mass *m*:

$$m\left(\frac{d^2\mathbf{r}}{dt^2}\right)_{inertial}=\mathbf{F}_{ext}$$

$$m\left(\frac{d^2\mathbf{r}}{dt^2}\right)_{body}=\mathbf{F}_{ext}-m\left(\frac{d^2\mathbf{a}}{dt^2}\right)_{inertial}-2m\boldsymbol{\omega}\times\left(\frac{d\mathbf{r}}{dt}\right)_{body}-m\frac{d\boldsymbol{\omega}}{dt}\times\mathbf{r}-m\boldsymbol{\omega}\times\boldsymbol{\omega}\times\mathbf{r}$$

Coriolis force

Centrifugal force

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Calculus of variation example for a pure integral functions

Find the function $y(x)$ which extremizes $S\left(\left\{y(x),\frac{dy}{dx}\right\},x\right)$

where $S\left(\left\{y(x),\frac{dy}{dx}\right\},x\right) \equiv \int_{x_i}^{x_f} f\left(\left\{y(x),\frac{dy}{dx}\right\},x\right)dx.$

Necessary condition: $\delta S = 0$

At any x, let $y(x) \to y(x) + \delta y(x)$

$$\frac{dy(x)}{dx} \to \frac{dy(x)}{dx} + \delta\frac{dy(x)}{dx}$$

Formally:

$$\delta S = \int_{x_i}^{x_f}\left[\left(\frac{\partial f}{\partial y}\right)_{x,\frac{dy}{dx}}\delta y + \left[\left(\frac{\partial f}{\partial(dy/dx)}\right)_{x,y}\delta\left(\frac{dy}{dx}\right)\right]\right]dx.$$

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Euler-Lagrange equation:

$$\Rightarrow\left(\frac{\partial f}{\partial y}\right)_{x,\frac{dy}{dx}} - \frac{d}{dx}\left[\left(\frac{\partial f}{\partial(dy/dx)}\right)_{x,y}\right] = 0 \quad \text{for all } x_i \le x \le x_f$$

Note that for $f\left(\left\{y(x),\frac{dy}{dx}\right\},x\right)$,

$$\frac{df}{dx} = \left(\frac{\partial f}{\partial y}\right)\frac{dy}{dx} + \left(\frac{\partial f}{\partial(dy/dx)}\right)\frac{d}{dx}\frac{dy}{dx} + \left(\frac{\partial f}{\partial x}\right)$$

$$= \left(\frac{d}{dx}\left(\frac{\partial f}{\partial(dy/dx)}\right)\right)\frac{dy}{dx} + \left(\frac{\partial f}{\partial(dy/dx)}\right)\frac{d}{dx}\frac{dy}{dx} + \left(\frac{\partial f}{\partial x}\right)$$

$$\Rightarrow \frac{d}{dx}\left(f - \frac{\partial f}{\partial(dy/dx)}\frac{dy}{dx}\right) = \left(\frac{\partial f}{\partial x}\right)$$

⇦ Alternate Euler-Lagrange equation

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Application to particle dynamics

$x \to t$ (time)

$y \to q$ (generalized coordinate)

$f \to L$ (Lagrangian)

$I \to S$ (action)

Denote: $\dot{q} \equiv \frac{dq}{dt}$

$$S = \int_{t_1}^{t_2} L(\{q,\dot{q}\};t)\,dt$$

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Now consider the Lagrangian defined to be:

$$L\left(\left\{y(t),\frac{dy}{dt}\right\},t\right)\equiv T-U$$

Kinetic energy (T) — Potential energy (U)

In our example:

$$L\left(\left\{y(t),\frac{dy}{dt}\right\},t\right)\equiv T-U=\frac{1}{2}m\left(\frac{dy}{dt}\right)^2-mgy$$

Hamilton's principle states:

$$S\equiv\int_{t_i}^{t_f}L\left(\left\{y(t),\frac{dy}{dt}\right\},t\right)dt \quad \text{is minimized for physical } y(t):$$

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Lagrangian function: $L(q,\dot{q},t)=T-U$

Euler-Lagrange equations: $\frac{d}{dt}\frac{\partial L}{\partial \dot{q}}-\frac{\partial L}{\partial q}=0$

$T \equiv$ Kinetic energy of system

$U \equiv$ Potential energy of system plus extra terms in the case of electric and/or magnetic fields

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

$$U=U_{mechanical}+U_{EM} \qquad U_{EM}=q\Phi(\mathbf{r},t)-\frac{q}{c}\dot{\mathbf{r}}\cdot\mathbf{A}(\mathbf{r},t)$$

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Recipe for constructing the Hamiltonian and analyzing the equations of motion

1. Construct Lagrangian function: $L=L(\{q_\sigma(t)\},\{\dot{q}_\sigma(t)\},t)$
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: $H=H(\{q_\sigma(t)\},\{p_\sigma(t)\},t)$
5. Analyze canonical equations of motion:

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

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Liouville's theorem:

Imagine a collection of particles obeying the Canonical equations of motion in phase space.

Let D denote the "distribution" of particles in phase space:

$$D = D(\{q_1 \cdots q_{3N}\}, \{p_1 \cdots p_{3N}\}, t)$$

Liouville's theorm shows that:

$$\frac{dD}{dt} = 0 \qquad \Rightarrow D \text{ is constant in time}$$

In statistical mechanics, we need to evaluate the probability of various configurations of particles. The fact that the density of particles in phase space is constant in time, implies that each point in phase space is equally probable and that the time average of the evolution of a system can be determined by an average of the system over phase space volume.

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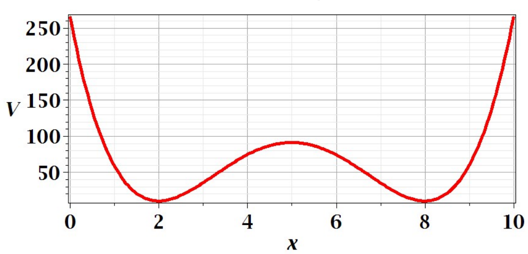
Motivation for studying small oscillations – many interacting systems have stable and meta-stable configurations which are well approximated by:

$$V(x) \approx V(x_{eq}) + \tfrac{1}{2}(x - x_{eq})^2 \left.\frac{d^2V}{dx^2}\right|_{x_{eq}} = V(x_{eq}) + \tfrac{1}{2}k(x - x_{eq})^2$$



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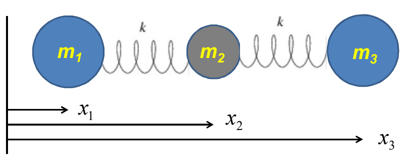
Example – linear molecule



$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2 - \frac{1}{2}k(x_2 - x_1 - \ell_{12})^2 - \frac{1}{2}k(x_3 - x_2 - \ell_{23})^2$$

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Let: $x_1 \to x_1 - x_1^0 \quad x_2 \to x_2 - x_1^0 - \ell_{12} \quad x_3 \to x_3 - x_1^0 - \ell_{12} - \ell_{23}$

$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2 - \frac{1}{2}k(x_2 - x_1)^2 - \frac{1}{2}k(x_3 - x_2)^2$$

Coupled equations of motion :

$$m_1\ddot{x}_1 = k(x_2 - x_1)$$
$$m_2\ddot{x}_2 = -k(x_2 - x_1) + k(x_3 - x_2) = k(x_1 - 2x_2 + x_3)$$
$$m_3\ddot{x}_3 = -k(x_3 - x_2)$$

Let $x_i(t) = X_i^\alpha e^{-i\omega_\alpha t}$

$$-\omega_\alpha^2 m_1 X_1^\alpha = k(X_2^\alpha - X_1^\alpha)$$
$$-\omega_\alpha^2 m_2 X_2^\alpha = k(X_1^\alpha - 2X_2^\alpha + X_3^\alpha)$$
$$-\omega_\alpha^2 m_3 X_3^\alpha = -k(X_3^\alpha - X_2^\alpha)$$

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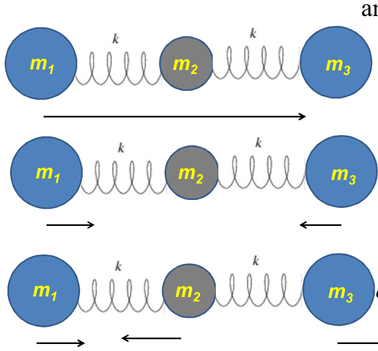
For $m_1 = m_3 \equiv m_O$

and $m_2 \equiv m_C$



$\omega_1 = 0$

$\omega_2 = \sqrt{\frac{k}{m_O}}$

$\omega_3 = \sqrt{\frac{k}{m_O} + \frac{2k}{m_C}}$

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General solution :

$$x_i(t) = \Re\left(\sum_\alpha C^\alpha X_i^\alpha e^{-i\omega_\alpha t}\right)$$

For example, normal mode amplitudes

C^α can be determined from initial conditions

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Digression:

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

Hermitian matrix : $H_{ij} = H^*_{ji}$

Theorem for Hermitian matrices :

λ_α have real values and $\mathbf{y}^H_\alpha \cdot \mathbf{y}_\beta = \delta_{\alpha\beta}$

Unitary matrix : $\mathbf{U}\mathbf{U}^H = \mathbf{I}$

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

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Digression on matrices -- continued

Eigenvalues of a matrix are "invariant" under a similarity transformation

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

Transformed matrix: $\mathbf{M}'\mathbf{y}'_\alpha = \lambda'_\alpha \mathbf{y}'_\alpha$

If $\mathbf{M}' = \mathbf{S}\mathbf{M}\mathbf{S}^{-1}$ then $\lambda'_\alpha = \lambda_\alpha$ and $\mathbf{S}^{-1}\mathbf{y}'_\alpha = \mathbf{y}_\alpha$

Proof $\mathbf{S}\mathbf{M}\mathbf{S}^{-1}\mathbf{y}'_\alpha = \lambda'_\alpha \mathbf{y}'_\alpha$

$\mathbf{M}\left(\mathbf{S}^{-1}\mathbf{y}'_\alpha\right) = \lambda'_\alpha \left(\mathbf{S}^{-1}\mathbf{y}'_\alpha\right)$

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Additional digression on matrix properties

Singular value decomposition

It is possible to factor any real matrix $\mathbf{A}$ into unitary matrices $\mathbf{V}$ and $\mathbf{U}$ together with positive diagonal matrix $\mathbf{\Sigma}$:

$$\mathbf{A} = \mathbf{U}\mathbf{\Sigma}\mathbf{V}^\mathbf{H}$$

$$\mathbf{\Sigma} = \begin{pmatrix} \sigma_1 & 0 & \cdots & 0 \\ 0 & \sigma_2 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & \sigma_N \end{pmatrix}$$

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Singular value decomposition -- continued

Consider using SVD to solve a singular linear algebra problem $\mathbf{AX} = \mathbf{B}$

$$\mathbf{A} = \mathbf{U}\Sigma\mathbf{V}^H$$

$$\mathbf{X} = \sum_{i \text{ for } \sigma_i > \varepsilon} \mathbf{v}_i \frac{\langle \mathbf{u}_i^H \mid \mathbf{B} \rangle}{\sigma_i}$$

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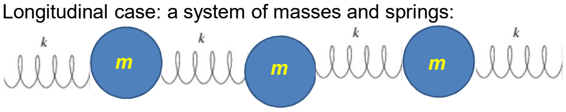
Longitudinal case: a system of masses and springs:



x_{i-1} x_i x_{i+1}

$$L = T - V = \frac{1}{2} m \sum_{i=0}^{\infty} \dot{x}_i^2 - \frac{1}{2} k \sum_{i=0}^{\infty} \left(x_{i+1} - x_i\right)^2$$

$$\Rightarrow m\ddot{x}_i = k\left(x_{i+1} - 2x_i + x_{i-1}\right)$$

Now imagine the continuum version of this system :

$$x_i(t) \Rightarrow \mu(x_i, t) \qquad \ddot{x}_i \Rightarrow \frac{\partial^2 \mu}{\partial t^2}$$

$$x_{i+1} - 2x_i + x_{i-1} \Rightarrow \frac{\partial^2 \mu}{\partial x^2}(\Delta x)^2$$

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Discrete equation : $m\ddot{x}_i = k\left(x_{i+1} - 2x_i + x_{i-1}\right)$

Continuum equation : $m \dfrac{\partial^2 \mu}{\partial t^2} = k(\Delta x)^2 \dfrac{\partial^2 \mu}{\partial x^2}$

$$\frac{\partial^2 \mu}{\partial t^2} = \left(\frac{k\Delta x}{m / \Delta x}\right) \frac{\partial^2 \mu}{\partial x^2}$$

system parameter with units of (velocity)^2

For transverse oscillations on a string with tension τ and mass/length σ:

$$\left(\frac{k\Delta x}{m / \Delta x}\right) \Rightarrow \frac{\tau}{\sigma}$$

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

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

Assume:

$$\mu(x,t) = f(x-ct) + g(x+ct)$$

then: $\mu(x,0) = \phi(x) = f(x) + g(x)$

$$\frac{\partial \mu}{\partial t}(x,0) = \psi(x) = -c\left(\frac{df(x)}{dx} - \frac{dg(x)}{dx}\right)$$

$$\Rightarrow f(x) - g(x) = -\frac{1}{c}\int^{x} \psi(x')dx'$$

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Solution -- continued: $\mu(x,t) = f(x-ct) + g(x+ct)$

then: $\mu(x,0) = \phi(x) = f(x) + g(x)$

$$\frac{\partial \mu}{\partial t}(x,0) = \psi(x) = -c\left(\frac{df(x)}{dx} - \frac{dg(x)}{dx}\right)$$

$$\Rightarrow f(x) - g(x) = -\frac{1}{c}\int^{x} \psi(x')dx'$$

For each x, find $f(x)$ and $g(x)$:

$$f(x) = \frac{1}{2}\left(\phi(x) - \frac{1}{c}\int^{x} \psi(x')dx'\right)$$

$$g(x) = \frac{1}{2}\left(\phi(x) + \frac{1}{c}\int^{x} \psi(x')dx'\right)$$

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

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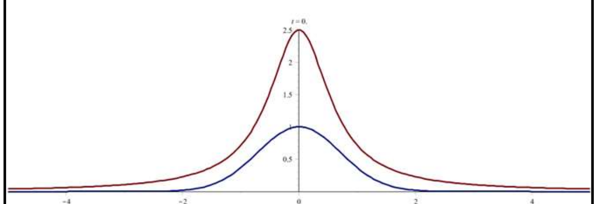
Example:

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

$$\Rightarrow \mu(\mathrm{x,t}) = \frac{1}{2}\left(e^{-(x+ct)^2/\sigma^2} + e^{-(x-ct)^2/\sigma^2}\right)$$



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