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

Plan for Lecture 16:

Review of Chap. 1-4,6

1. **Scattering theory**
2. **Rotation reference frames**
3. **Calculus of variation**
4. **Legrangian and Hamiltonian formalisms**
5. **Normal modes of vibration**

Course schedule

(Preliminary schedule -- subject to frequent adjustment.)

	Date	F&W Reading	Topic	Assignment	Due
1	Mon, 8/27/2018	Chap. 1	Introduction	#1	9/7/2018
	Wed, 8/29/2018	No class			
2	Fri, 8/31/2018	Chap. 1	Scattering theory	#2	9/7/2018
3	Mon, 9/03/2018	Chap. 1	Scattering theory		
4	Wed, 9/05/2018	Chap. 1	Scattering theory	#3	9/10/2018
5	Fri, 9/07/2018	Chap. 2	Non-inertial coordinate systems	#4	9/12/2018
6	Mon, 9/10/2018	Chap. 3	Calculus of Variation	#5	9/12/2018
7	Wed, 9/12/2018	Chap. 3	Calculus of Variation	#6	9/17/2018
	Fri, 9/14/2018	No class	University closed due to weather.		
8	Mon, 9/17/2018	Chap. 3	Lagrangian Mechanics	#7	9/19/2018
9	Wed, 9/19/2018	Chap. 3 and 6	Lagrangian Mechanics and constraints	#8	9/24/2018
10	Fri, 9/21/2018	Chap. 3 and 6	Constants of the motion		
11	Mon, 9/24/2018	Chap. 3 and 6	Hamiltonian formalism	#9	9/28/2018
12	Wed, 9/26/2018	Chap. 3 and 6	Liouville theorem	#10	10/3/2018
13	Fri, 9/28/2018	Chap. 3 and 6	Canonical transformations		
14	Mon, 10/1/2018	Chap. 4	Small oscillations about equilibrium	#11	10/5/2018
15	Wed, 10/3/28/2018	Chap. 4	Normal modes of vibration		
16	Fri, 10/5/2018	Chap. 1-4, 6	Review		
17	Mon, 10/8/2018	Chap. 7	Strings		

Scattering theory

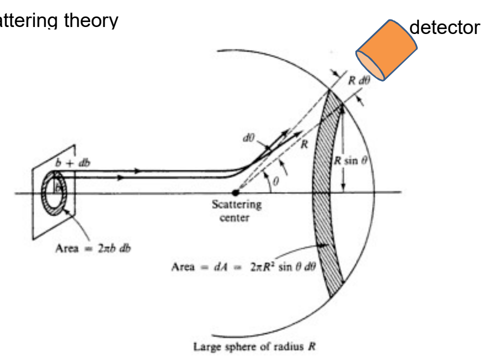
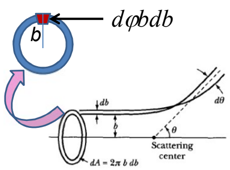


Figure 5.5 The scattering problem and relation of cross section to impact parameter.

Differential cross section

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

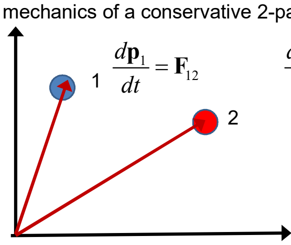
$$= \text{ Area of incident beam that is scattered into detector at angle } \theta$$



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

Figure from Marion & Thorton, Classical Dynamics

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



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

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

Relationship between center of mass and laboratory frames of reference

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

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

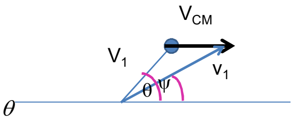
$$m_1\dot{\mathbf{r}}_1 + m_2\dot{\mathbf{r}}_2 = \left(m_1 + m_2\right)\dot{\mathbf{R}}_{CM} = \left(m_1 + m_2\right)\mathbf{V}_{CM}$$

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

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

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

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

Conserved energy in CM frame

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

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 **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

Calculus of variation example for a pure integral functions

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

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

Necessary condition : $\delta L = 0$

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

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

Formally :

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

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

Application to particle dynamics

$x \rightarrow t$ (time)

$y \rightarrow q$ (generalized coordinate)

$f \rightarrow L$ (Lagrangian)

$I \rightarrow S$ (action)

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

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

Now consider the Lagrangian defined to be:

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

Kinetic energy

Potential energy

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:

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

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

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

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

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 :

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

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:

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

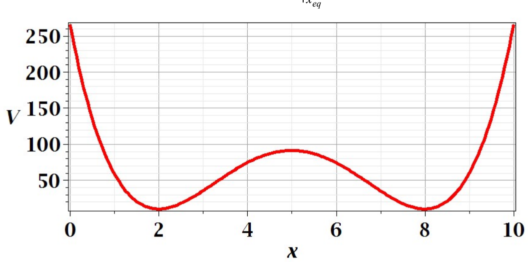
Liouville's theorm shows that:

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

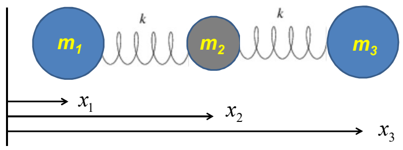
In statistical mechanics, we need to evaluate the probability of various configurations of particles. The fact that the density of particles in phase space is constant in time, implies that each point in phase space is equally probable and that the time average of the evolution of a system can be determined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

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

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



Example – linear molecule



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

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

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

Coupled equations of motion :

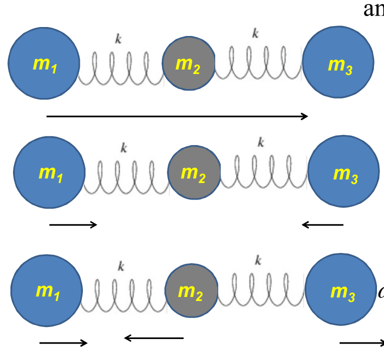
$$m_1\ddot{x}_1 = k(x_2 - x_1)$$
$$m_2\ddot{x}_2 = -k(x_2 - x_1) + k(x_3 - x_2) = k(x_1 - 2x_2 + x_3)$$
$$m_3\ddot{x}_3 = -k(x_3 - x_2)$$

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

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

For $m_1 = m_3 \equiv m_O$

and $m_2 \equiv m_C$



$\omega_1 = 0$

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

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

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

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 $\mathbf{y}_\alpha^H \cdot \mathbf{y}_\beta = \delta_{\alpha\beta}$

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

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

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

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

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 $\mathbf{\Sigma}$:

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

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

Singular value decomposition -- continued

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

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

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