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

Notes for Lecture 17 – Chap. 1-6 (F & W)

Review

1. Some advice about problem solving
2. Solutions of selected problems
3. Systematic review

	Date	F&W	Topic	HW
1	Mon, 8/26/2024		Introduction and overview	#1
2	Wed, 8/28/2024	Chap. 3(17)	Calculus of variation	#2
3	Fri, 8/30/2024	Chap. 3(17)	Calculus of variation	#3
4	Mon, 9/02/2024	Chap. 3	Lagrangian equations of motion	#4
5	Wed, 9/04/2024	Chap. 3 & 6	Lagrangian equations of motion	#5
6	Fri, 9/06/2024	Chap. 3 & 6	Lagrangian equations of motion	#6
7	Mon, 9/09/2024	Chap. 3 & 6	Lagrangian to Hamiltonian formalism	#7
8	Wed, 9/11/2024	Chap. 3 & 6	Phase space	#8
9	Fri, 9/13/2024	Chap. 3 & 6	Canonical Transformations	
10	Mon, 9/16/2024	Chap. 5	Dynamics of rigid bodies	#9
11	Wed, 9/18/2024	Chap. 5	Dynamics of rigid bodies	#10
12	Fri, 9/20/2024	Chap. 5	Dynamics of rigid bodies	#11
13	Mon, 9/23/2024	Chap. 1	Scattering analysis	#12
14	Wed, 9/25/2024	Chap. 1	Scattering analysis	#13
15	Fri, 9/27/2024	Chap. 1	Scattering analysis	#14
16	Mon, 9/30/2024	Chap. 4	Small oscillations near equilibrium	
17	Wed, 10/2/2024	Chap. 1-6	Review	THE-10/3-10/24
18	Fri, 10/4/2024	Chap. 4	Normal mode analysis	THE-10/3-10/24

Physics Colloquium

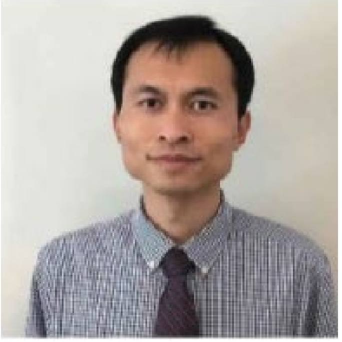
- Thursday -

October 3, 2024

In situ Vibrational Spectroscopic Studies of Chemical and Molecular Interactions in Metal-Organic Frameworks

4 PM
Olin 101

Precisely characterizing the interactions of gaseous molecules in nanoporous materials such as metal-organic frameworks (MOFs) is challenging yet crucial to understand guest adsorption behaviours and host structure features of importance for applications such as gas storage, separation, purification, and catalysis. Such guest-host and guest-guest interactions range from strong chemical reactive binding to weak physical non-reactive (e.g., van der Waals) ones, which complicate the measurement and analysis. In our studies we show that vibrational characterization, particularly infrared spectroscopy conducted under *in situ* conditions, is arguably one of the most discriminating tools to probe the nature and strength of these interactions and reveal mechanistic information pertaining to kinetics and energetics of adsorption processes. We first examine how H_2O reactively interacts with three types of prototypical MOF compounds: 1) MOFs with saturated metal canters, 2) MOFs with unsaturated metal centres, and 3) MOFs with defects, and derive a clear microscopic view about the degradation pathways of some complex MOF structures under moisture. We then show results for co-adsorption of non-reactive species such as CO_2, CO, C_2H_2, C_2H_4 in several benchmark compounds. Such processes remain poorly understood due to the difficulties inherent in current characterization methods and we establish several unexpected findings with respect to the principles governing co-adsorption. For example, binding energy alone is not a sufficient indicator for prediction of molecular exchange and stability—instead, kinetics can govern adsorption in nanoconfined spaces. We also find an unusual synergistic effect involving co-adsorption of NH_3 and H_2O with a variety of small



Professor Kui Tan

University of North Texas

Comments about the exam

Will be available tomorrow (10/3/2024)

Due --

Sun	Mon	Tue	Wed	Thu	Fri	Sat
29	30	1	2	3	4	5
6	7	8	9	10	11	12

- It must be your own work, under the honor code
- Please make sure that the grader can read your answers.
- Grading is based on the correct answer AND the correct reasoning to arrive at the correct answer. Full credit is obtained only with both. Partial credit also benefits from clear reasoning and results.
- Please meet with me **only** (in person or by email) if you have questions about the exam.

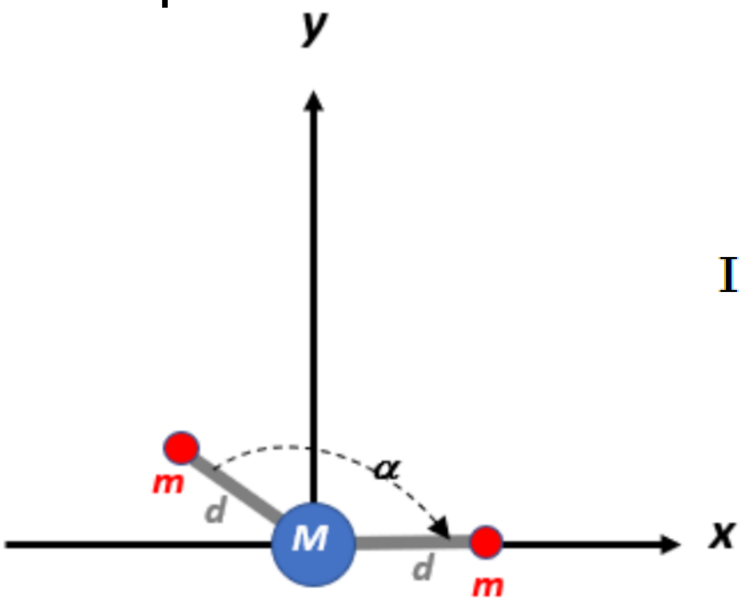
Comments on exam

- The purpose of the exam is to help you with your understanding of the material
- In accordance with the honor code, the solutions you hand in must be your own work.   That is, if you have any questions, please consult with me, **but no one else.**
- You will get credit for the reasoning and derivations as well as for the right answer. You may use software such as including Mathematica, Maple, etc. as long as you include all input/output with your exam.
- This is an open “book” exam which means that you can consult textbooks and lecture notes as long as you cite themIt is often helpful approach problems in more than one way – recalling that undergraduate physics is still true.

Steps for tackling a problem –

1. What are the basic concepts that apply to this problem?
2. Write down the fundamental equations specific to this situation.
3. Solve.
4. Check.

Example Problem -- HW #5



$$\mathbf{I} = md^2 \begin{pmatrix} \sin^2\alpha & -\cos\alpha\sin\alpha & 0 \\ -\cos\alpha\sin\alpha & 1+\cos^2\alpha & 0 \\ 0 & 0 & 2 \end{pmatrix}$$

1. The figure above shows a rigid 3 atom molecule placed in the *x*-*y* plane as shown. Assume that the rigid bonds are massless.
   a. Find the moment of inertia tensor in the given coordinate system placed of mass *M* in terms of the atom masses, bond lengths *d*, and angle α.
   b. Find the principal moments moments of inertia I_1, I_2, I_3 and the corresponding principal axes.

$$I_1 = md^2(1-\cos\alpha) \quad I_2 = md^2(1+\cos\alpha) \quad I_3 = 2md.$$

Example solution – Problems 5&7

For given constants $m, q, c, E_0, B_0,$ consider the Lagrangian

$$L(x,y,z,\dot{x},\dot{y},\dot{z}) = \frac{1}{2}m\left(\dot{x}^2+\dot{y}^2+\dot{z}^2\right) - \frac{q}{c}\dot{z}\left(E_0ct+B_0x\right)$$

Initial conditions: $x(t)=0, y(t)=0, z(t)=0$

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

Find Hamiltonian and solve the canonical equations of motion.

$$p_x = \frac{\partial L}{\partial \dot{x}} = m\dot{x} \qquad p_y = \frac{\partial L}{\partial \dot{y}} = m\dot{y}$$

$$p_z = \frac{\partial L}{\partial \dot{z}} = m\dot{z} - \frac{q}{c}\left(E_0ct+B_0x\right)$$

$$H = p_x\dot{x} + p_y\dot{y} + p_z\dot{z} - L = \frac{1}{2}m\left(\dot{x}^2+\dot{y}^2+\dot{z}^2\right)$$

$$H\left(x,y,z,p_x,p_y,p_z,t\right) = \frac{p_x^2}{2m} + \frac{p_y^2}{2m} + \frac{\left(p_z - \frac{q}{c}\left(E_0ct+B_0x\right)\right)^2}{2m}$$

$$H\left(x,y,z,p_x,p_y,p_z,t\right)=\frac{p_x^2}{2m}+\frac{p_y^2}{2m}+\frac{\left(p_z-\frac{q}{c}\left(E_0ct+B_0x\right)\right)^2}{2m}$$

Some of the canonical equations:

$$\dot{p}_z=-\frac{\partial H}{\partial z}=0 \quad \Rightarrow p_z=\text{constant}=\left(m\dot{z}-\frac{q}{c}\left(E_0ct+B_0x\right)\right)_{t=0}=0$$

$$\dot{z}=\frac{\partial H}{\partial p_z}=\frac{q}{mc}\left(E_0ct+B_0x\right)$$

$$\dot{p}_x=-\frac{\partial H}{\partial x}=-\frac{q^2B_0}{mc^2}\left(E_0ct+B_0x\right)$$

$$\dot{x}=\frac{\partial H}{\partial p_x}=\frac{p_x}{m} \qquad \Rightarrow \ddot{x}=\frac{\dot{p}_x}{m}=-\frac{q^2B_0}{m^2c^2}\left(E_0ct+B_0x\right)$$

When the dust clears -- $x(t)=\frac{E_0c}{B_0}\left(\frac{mc}{qB_0}\sin\left(\frac{qB_0}{mc}t\right)-t\right)$

$$z(t)=\frac{E_0c}{B_0}\frac{mc}{qB_0}\left(-\cos\left(\frac{qB_0}{mc}t\right)+1\right)$$

PHY 711 – Assignment #12

Assigned: 09/23/2024   Due: 9/30/2024

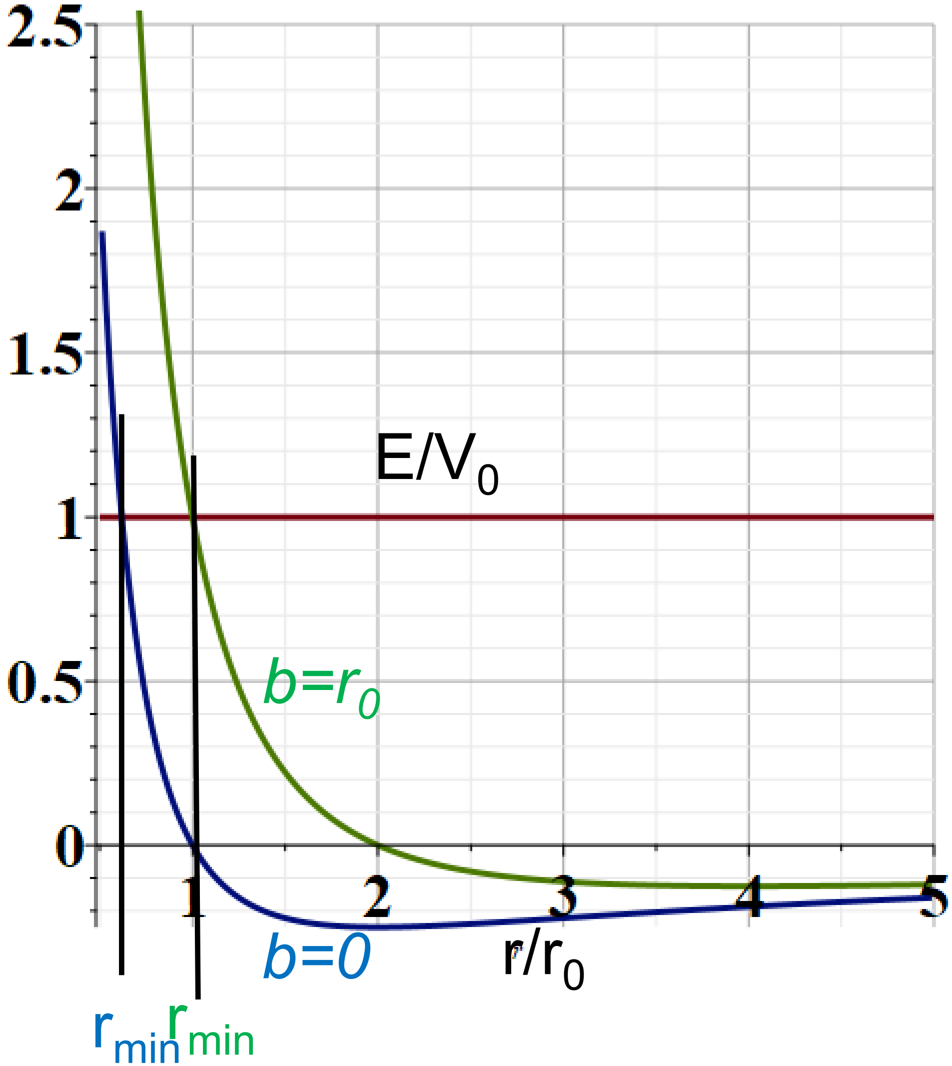
1. Consider a particle of mass m moving in the vicinity of another particle of mass M, initially at rest, where $m << M$. The particles interact with a conservative central potential of the form

$$V(r) = V_0 \left(\left(\frac{r_0}{r}\right)^2 - \left(\frac{r_0}{r}\right) \right),$$

where r denotes the magnitude of the particle separation and V_0 and r_0 denote energy and length constants, respectively. The total energy of the system E is constant and $E = V_0$.

   (a) First consider the case where the impact parameter $b = 0$. Find the distance of closest approach of the particles.

   (b) Now consider the case where the impact parameter $b = r_0$. Find the distance of closest approach of the particles.



$$V(r) = V_0\left(\left(\frac{r_0}{r}\right)^2 - \left(\frac{r_0}{r}\right)\right)$$

$$E = \frac{1}{2}m\dot{r}^2 + V(r) + \frac{b^2 E}{r^2}$$

PHY 711 -- Assignment #14

Assigned: 9/27/2024 Due: 9/30/2024

Continue reading Chapter 1 in **Fetter & Walecka**.

- Work Problem #1.16 at the end of Chapter 1 in **Fetter and Walecka**. Note that you might want to use the equation in FW #1.15 or the equivalent equation derived in class.

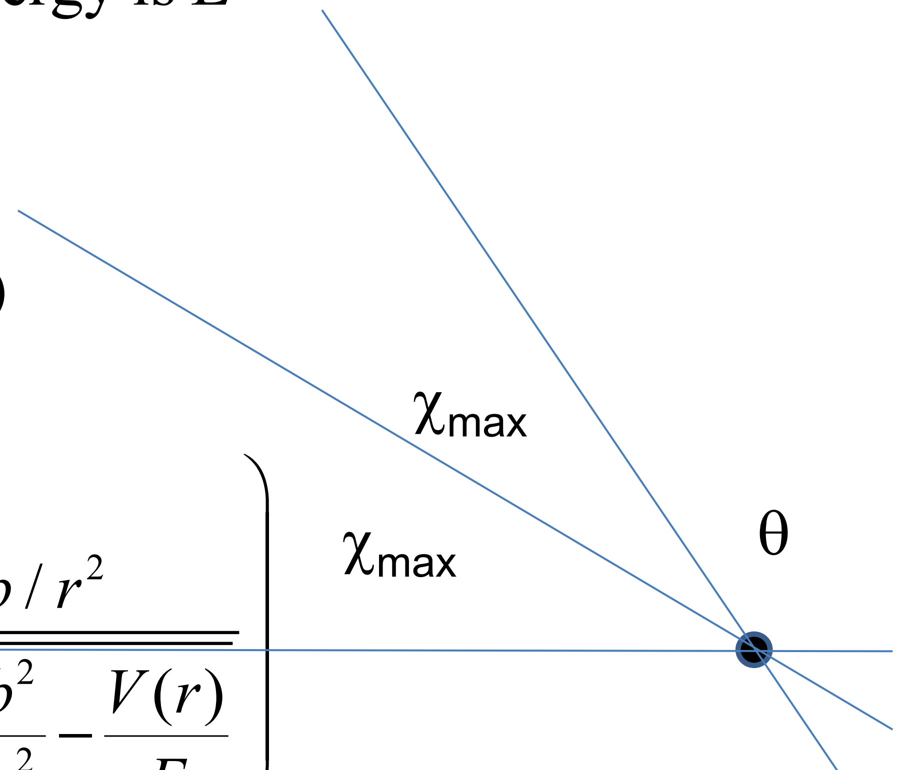
In this case, $V(r) = \frac{\gamma}{r^2}$ and energy is E

$$E = \frac{1}{2}m\dot{r}^2 + V(r) + \frac{b^2 E}{r^2}$$

can be analyzed from $r(t) \rightarrow r(\chi)$

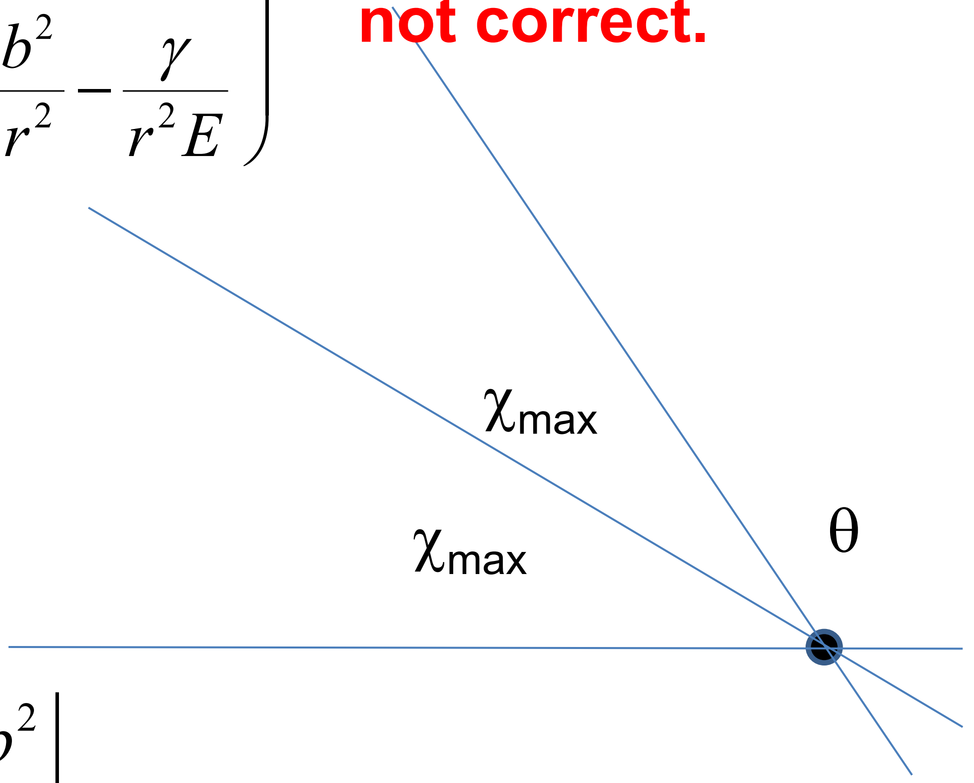
$$2\chi_{max} + \theta = \pi$$

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



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

Lecture 15 has the opposite sign and is not correct.

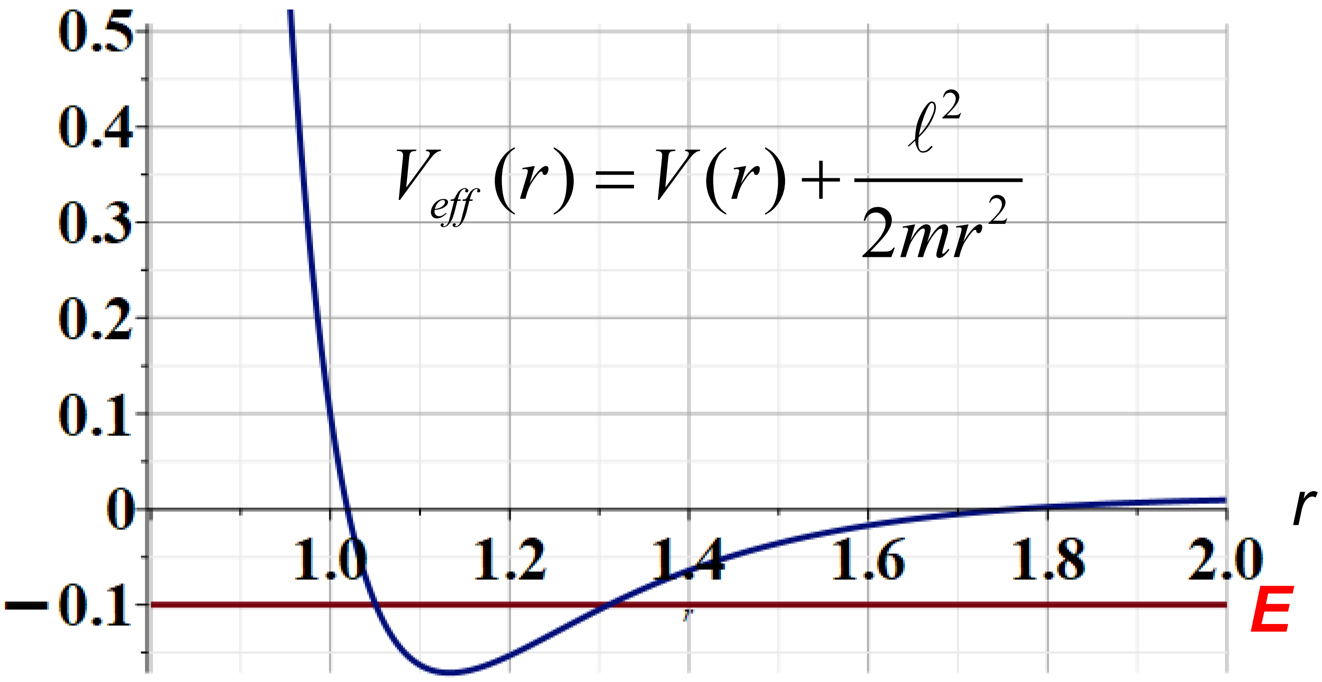


$$b^2 = \frac{E}{\gamma} \frac{\left(1 - \frac{\theta}{\pi}\right)^2}{\frac{\theta}{\pi}\left(2 - \frac{\theta}{\pi}\right)}$$

$$\frac{d\sigma}{d\Omega} = \frac{b}{\sin\theta}\left|\frac{db}{d\theta}\right| = \frac{1}{2\sin\theta}\left|\frac{db^2}{d\theta}\right|$$

Systematic review

1. Basic principles
   Scattering analysis
   Mechanics of central forces

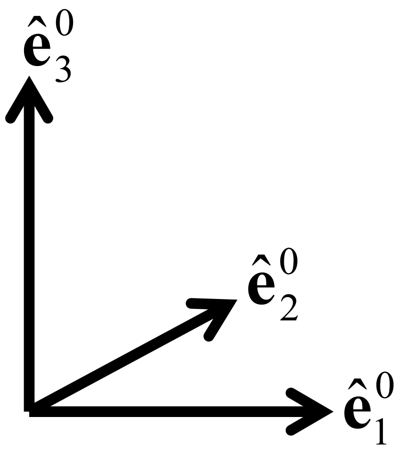


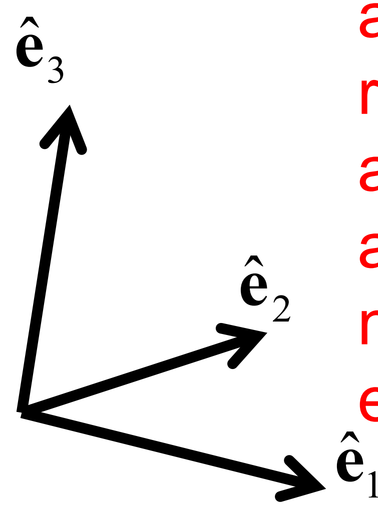
Systematic review

2. Accelerated Coordinate Systems

Physical laws as described in non-inertial coordinate systems

- Newton's laws are formulated in an inertial frame of reference $\left\{ \hat{\mathbf{e}}_i^0 \right\}$
- For some problems, it is convenient to transform the the equations into a non-inertial coordinate system $\left\{\hat{\mathbf{e}}_i\left(t\right)\right\}$





Note that in addition to rotation, linear acceleration can also contribute to non-inertial effects.

Comparison of analysis in "inertial frame" versus "non-inertial frame"

Denote by $\hat{\mathbf{e}}_i^0$ an fixed coordinate system in 3 orthogonal directions

Denote by $\hat{\mathbf{e}}_i$ a moving coordinate system in 3 orthogonal directions

$$\mathbf{V} = \sum_{i=1}^{3} V_i^0 \hat{\mathbf{e}}_i^0 = \sum_{i=1}^{3} V_i \hat{\mathbf{e}}_i$$

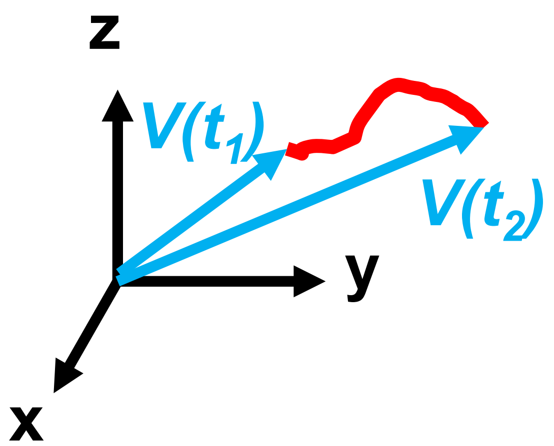
$$\left(\frac{d\mathbf{V}}{dt}\right)_{inertial} = \sum_{i=1}^{3} \frac{dV_i^0}{dt} \hat{\mathbf{e}}_i^0 = \sum_{i=1}^{3} \frac{dV_i}{dt} \hat{\mathbf{e}}_i + \sum_{i=1}^{3} V_i \frac{d\hat{\mathbf{e}}_i}{dt}$$

Define: $$\left(\frac{d\mathbf{V}}{dt}\right)_{body} \equiv \sum_{i=1}^{3} \frac{dV_i}{dt} \hat{\mathbf{e}}_i$$

This represents the time rate of change of V measured within the e frame.

$$\Rightarrow \left(\frac{d\mathbf{V}}{dt}\right)_{inertial} = \left(\frac{d\mathbf{V}}{dt}\right)_{body} + \sum_{i=1}^{3} V_i \frac{d\hat{\mathbf{e}}_i}{dt}$$

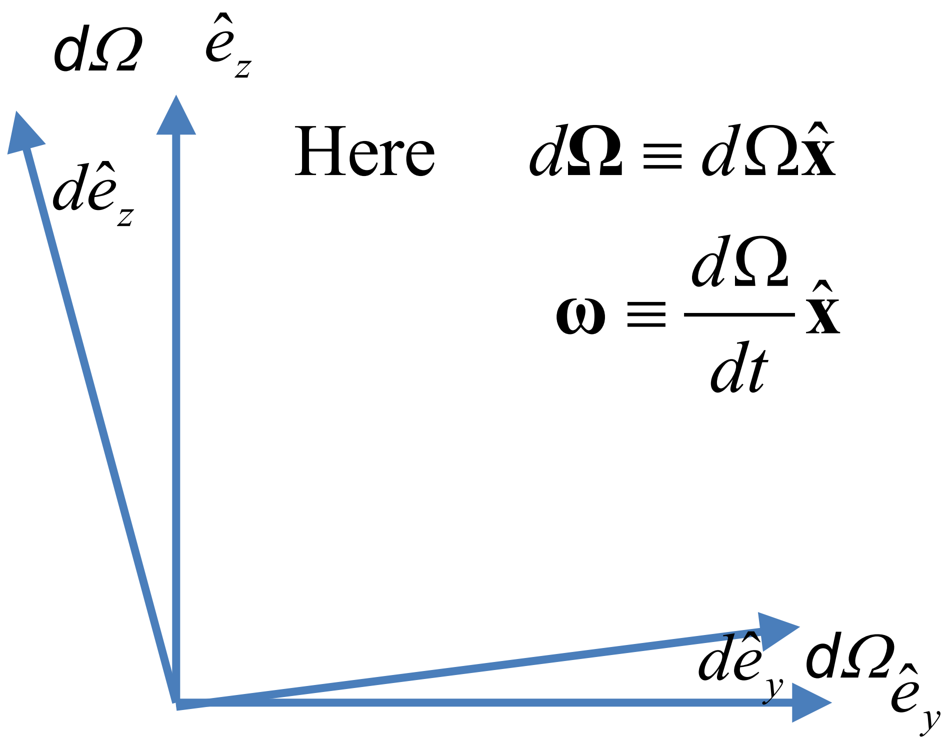
e^0 example



$$\frac{d\mathbf{V}(t)}{dt} = \frac{dV_x^0(t)}{dt}\hat{\mathbf{x}} + \frac{dV_y^0(t)}{dt}\hat{\mathbf{y}} + \frac{dV_z^0(t)}{dt}\hat{\mathbf{z}}$$

e example – same motion described in moving coordinate system.

Properties of the frame motion (rotation only):



Here $d\mathbf{\Omega} \equiv d\Omega \hat{\mathbf{x}}$

$$\boldsymbol{\omega} \equiv \frac{d\Omega}{dt}\hat{\mathbf{x}}$$

$$d\hat{e}_y = d\Omega \hat{e}_z$$

$$d\hat{e}_z = -d\Omega \hat{e}_y$$

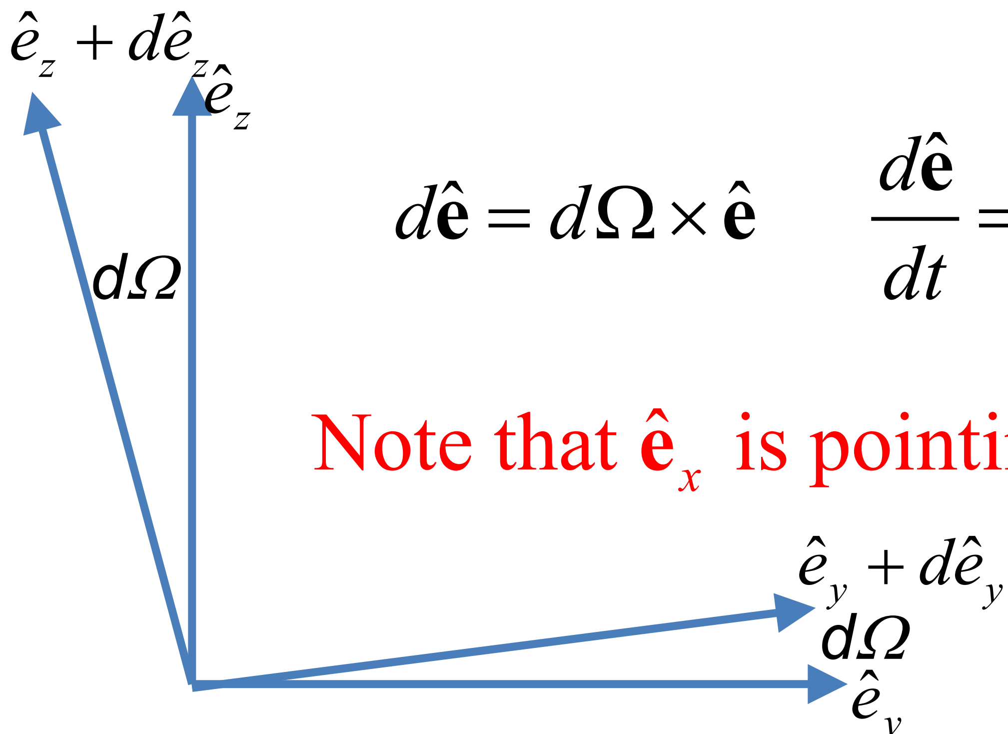
$$\Rightarrow d\hat{\mathbf{e}} = d\mathbf{\Omega} \times \hat{\mathbf{e}}$$

$$\frac{d\hat{\mathbf{e}}}{dt} = \frac{d\mathbf{\Omega}}{dt} \times \hat{\mathbf{e}}$$

$$\frac{d\hat{\mathbf{e}}}{dt} = \boldsymbol{\omega} \times \hat{\mathbf{e}}$$

Note that the coordinate $\hat{\mathbf{e}}_x$ is pointing out of the screen.

Properties of the frame motion (rotation only):



$$d\hat{\mathbf{e}} = d\boldsymbol{\Omega} \times \hat{\mathbf{e}} \qquad \frac{d\hat{\mathbf{e}}}{dt} = \frac{d\boldsymbol{\Omega}}{dt} \times \hat{\mathbf{e}} \qquad \frac{d\hat{\mathbf{e}}}{dt} = \boldsymbol{\omega} \times \hat{\mathbf{e}}$$

Note that $\hat{\mathbf{e}}_x$ is pointing out of the screen.

rotation matrix

Rotation about x-axis:

$$\begin{pmatrix} e_y \\ e_z \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} e_y \\ e_z \end{pmatrix} \qquad \begin{pmatrix} e_y + de_y \\ e_z + de_z \end{pmatrix} = \begin{pmatrix} \cos(d\Omega) & \sin(d\Omega) \\ -\sin(d\Omega) & \cos(d\Omega) \end{pmatrix} \begin{pmatrix} e_y \\ e_z \end{pmatrix}$$

$$\begin{pmatrix} de_y \\ de_z \end{pmatrix} = \begin{pmatrix} \cos(d\Omega) - 1 & \sin(d\Omega) \\ -\sin(d\Omega) & \cos(d\Omega) - 1 \end{pmatrix} \begin{pmatrix} e_y \\ e_z \end{pmatrix} \approx \begin{pmatrix} 0 & d\Omega \\ -d\Omega & 0 \end{pmatrix} \begin{pmatrix} e_y \\ e_z \end{pmatrix}$$

More details

Rotation about x-axis:

$$\begin{pmatrix} e_y \\ e_z \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} e_y \\ e_z \end{pmatrix} \qquad \begin{pmatrix} e_y + de_y \\ e_z + de_z \end{pmatrix} = \begin{pmatrix} \cos(d\Omega) & \sin(d\Omega) \\ -\sin(d\Omega) & \cos(d\Omega) \end{pmatrix} \begin{pmatrix} e_y \\ e_z \end{pmatrix}$$

$$\begin{pmatrix} de_y \\ de_z \end{pmatrix} = \begin{pmatrix} \cos(d\Omega)-1 & \sin(d\Omega) \\ -\sin(d\Omega) & \cos(d\Omega)-1 \end{pmatrix} \begin{pmatrix} e_y \\ e_z \end{pmatrix} \approx \begin{pmatrix} 0 & d\Omega \\ -d\Omega & 0 \end{pmatrix} \begin{pmatrix} e_y \\ e_z \end{pmatrix}$$

$$e_y + de_y = \cos(d\Omega)e_y + \sin(d\Omega)e_z$$

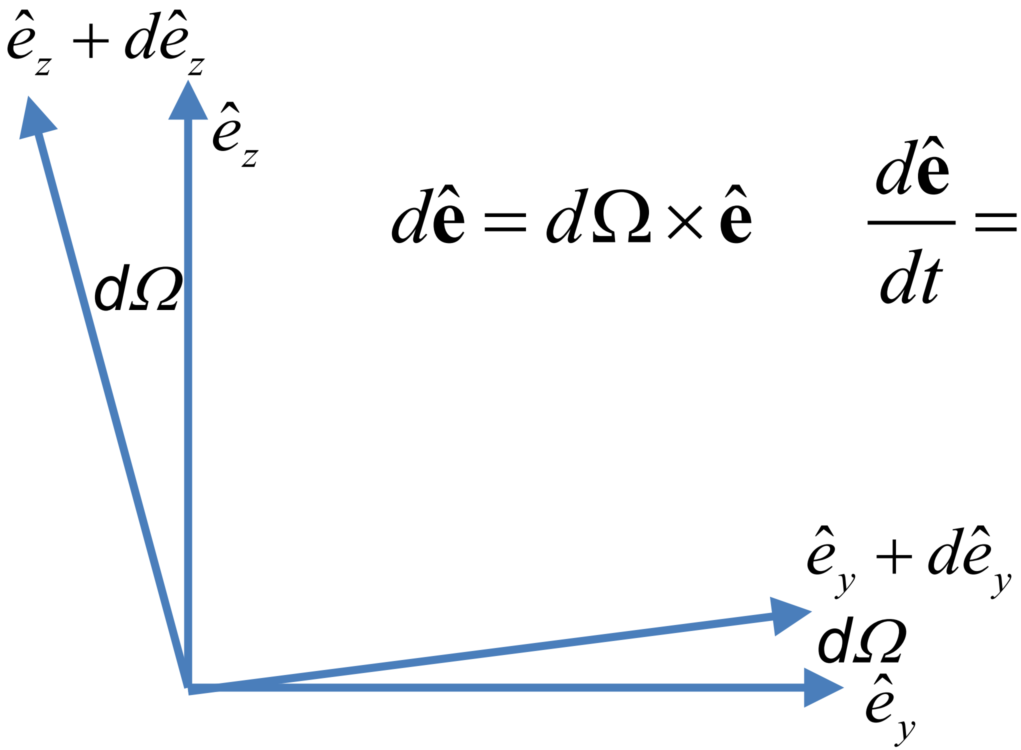
$$e_z + de_z = -\sin(d\Omega)e_y + \cos(d\Omega)e_z$$

Taylor's series

$$f(x_0 + dx) = f(x_0) + dx \left.\frac{df}{dx}\right|_{x_0} + \frac{1}{2}(dx)^2 \left.\frac{d^2 f}{dx^2}\right|_{x_0} + ...$$

$$\sin(dx) = dx - \frac{1}{6}(dx)^3 .... \approx dx \qquad \cos(dx) = 1 - \frac{1}{2}(dx)^2 .... \approx 1$$

Properties of the frame motion (rotation only):



$$d\hat{\mathbf{e}} = d\Omega \times \hat{\mathbf{e}} \qquad \frac{d\hat{\mathbf{e}}}{dt} = \frac{d\Omega}{dt} \times \hat{\mathbf{e}} \qquad \frac{d\hat{\mathbf{e}}}{dt} = \boldsymbol{\omega} \times \hat{\mathbf{e}}$$

Rotation about x-axis:

$$\begin{pmatrix} de_y \\ de_z \end{pmatrix} \approx \begin{pmatrix} 0 & d\Omega \\ -d\Omega & 0 \end{pmatrix} \begin{pmatrix} e_y \\ e_z \end{pmatrix} = d\Omega e_z \hat{\mathbf{y}} - d\Omega e_y \hat{\mathbf{z}} = d\Omega \hat{\mathbf{x}} \times \hat{\mathbf{e}}$$

Define axial vectors $\mathbf{d\Omega} \equiv d\Omega \hat{\mathbf{x}}$ also $\boldsymbol{\omega} = \omega \hat{\mathbf{x}}$

Properties of the frame motion (rotation only) -- continued

$$\left(\frac{d\mathbf{V}}{dt}\right)_{inertial} = \left(\frac{d\mathbf{V}}{dt}\right)_{body} + \sum_{i=1}^{3} V_i \frac{d\hat{\mathbf{e}}_i}{dt}$$

$$\left(\frac{d\mathbf{V}}{dt}\right)_{inertial} = \left(\frac{d\mathbf{V}}{dt}\right)_{body} + \boldsymbol{\omega}\times\mathbf{V} = \left(\left(\frac{d}{dt}\right)_{body} + \boldsymbol{\omega}\times\right)\mathbf{V}$$

Effects on 2nd time derivative -- acceleration (rotation only):

$$\left(\frac{d}{dt}\frac{d\mathbf{V}}{dt}\right)_{inertial} = \left(\left(\frac{d}{dt}\right)_{body} + \boldsymbol{\omega}\times\right)\left\{\left(\frac{d\mathbf{V}}{dt}\right)_{body} + \boldsymbol{\omega}\times\mathbf{V}\right\}$$

$$\left(\frac{d^2\mathbf{V}}{dt^2}\right)_{inertial} = \left(\frac{d^2\mathbf{V}}{dt^2}\right)_{body} + 2\boldsymbol{\omega}\times\left(\frac{d\mathbf{V}}{dt}\right)_{body} + \frac{d\boldsymbol{\omega}}{dt}\times\mathbf{V} + \boldsymbol{\omega}\times\boldsymbol{\omega}\times\mathbf{V}$$

Application of Newton's laws in a coordinate system which has an angular velocity $\boldsymbol{\omega}$ and linear acceleration **a**

(Here we generalize previous case to add linear acceleration **a**.)

Newton's laws; Let **r** denote the position of particle of mass *m*:

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

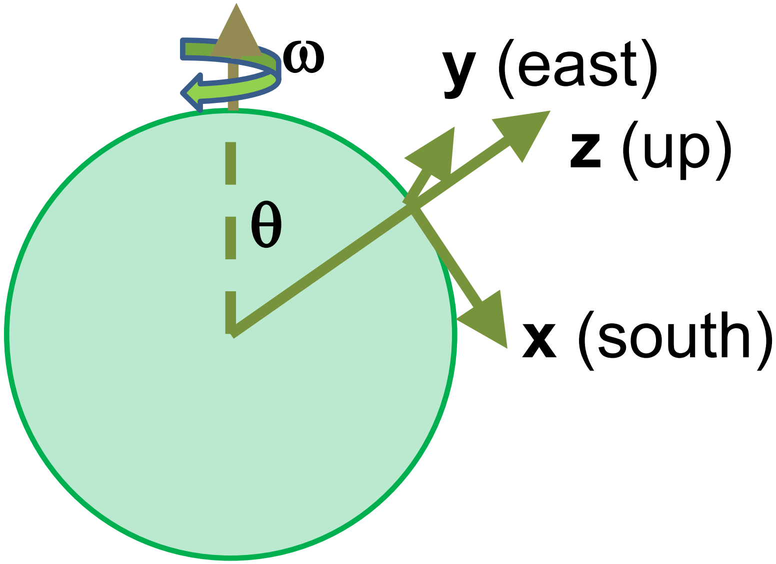
$$m\left(\frac{d^2\mathbf{r}}{dt^2}\right)_{inertial} = m\left(\mathbf{a} + \left(\frac{d^2\mathbf{r}}{dt^2}\right)_{body} + 2\boldsymbol{\omega}\times\left(\frac{d\mathbf{r}}{dt}\right)_{body} + \frac{d\boldsymbol{\omega}}{dt}\times\mathbf{r} + \boldsymbol{\omega}\times\boldsymbol{\omega}\times\mathbf{r}\right)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

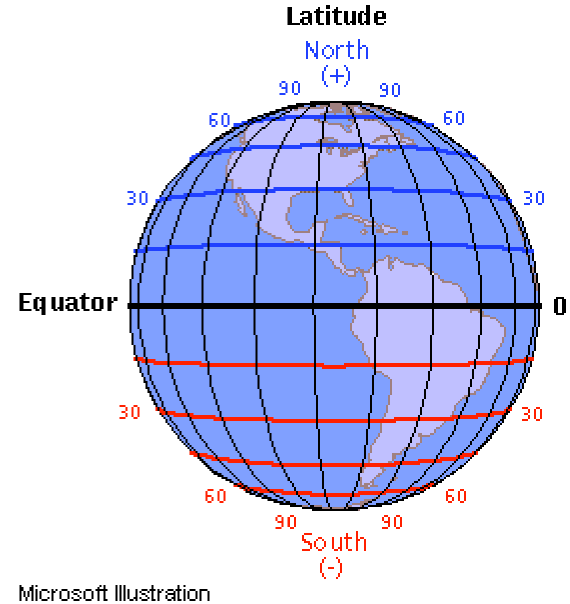
Rearranging to find the effective acceleration within the non-inertial frame --

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

Coriolis force

Centrifugal force





$$\omega_\perp \equiv \omega_0 \cos\theta$$

Motion of a Foucoult Pendulum

$$x(t) = X_0 \cos\left(\sqrt{\frac{g}{\ell}}t\right)\cos\left(\omega_\perp t\right)$$

$$y(t) = -X_0 \cos\left(\sqrt{\frac{g}{\ell}}t\right)\sin\left(\omega_\perp t\right)$$

Chapter 3 -- Calculus of variation –

Consider a family of functions $y(x)$, with fixed end points

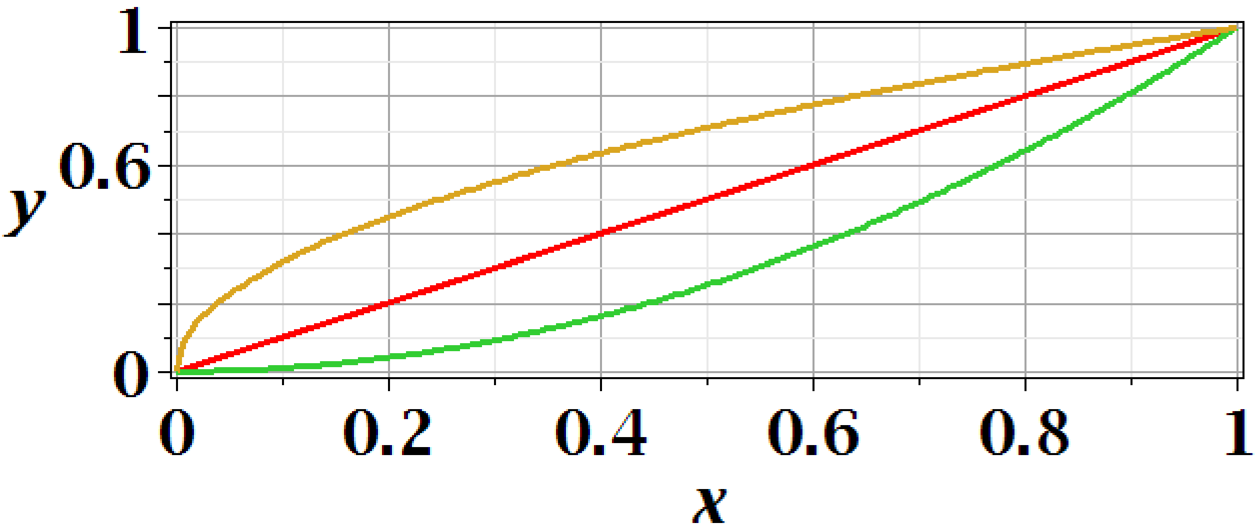
$y(x_i) = y_i$ and $y(x_f) = y_f$ and an integral form $L\left(\left\{y(x), \frac{dy}{dx}\right\}, x\right)$.

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

Necessary condition: $\delta L = 0$

Example:

$$L = \int_{(0,0)}^{1,1} \sqrt{(dx)^2 + (dy)^2}$$



After some derivations, we find

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

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

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

Note that this is a
"total" derivative

Summary --

Optimizing $I=\int_{x_i}^{x_f} f(y,\frac{dy}{dx},x)dx$ -- for fixed $y(x_i)\equiv y_i$ and $y(x_f)\equiv y_f$

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

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

Euler-Lagrange equation

Question -- what would be the Euler-Lagrange-type relation for

optimizing $I=\int_{x_i}^{x_f} f(y,\frac{dy}{dx},\frac{d^2y}{dx^2},x)dx$ -- for fixed $y(x_i)\equiv y_i$ and $y(x_f)\equiv y_f$

We are now going to shift notation in order to apply the calculus of variation formalism to Hamilton's principle and Lagrangian mechanics.

$$x \rightarrow t$$

$$y(x) \rightarrow q(t)$$

$$\frac{dy}{dx} \rightarrow \dot{q}(t)$$

Application to particle dynamics

Hamilton's principle states that the dynamical trajectory of a system is given by the path that extremizes the action integral

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

Simple example: vertical trajectory of particle of mass *m* subject to constant downward acceleration *a*=-*g.*

Newton's formulation: $m\frac{d^2y}{dt^2} = -mg$

Resultant trajectory: $y(t) = y_i + v_i t - \frac{1}{2}gt^2$

Lagrangian for this case:

$$L = \frac{1}{2}m\left(\frac{dy}{dt}\right)^2 - mgy$$

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:

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

Condition for minimizing the action in example:

$$S \equiv \int_{t_i}^{t_f} \left(\frac{1}{2} m \left(\frac{dy}{dt} \right)^2 - mgy \right) dt$$

Euler-Lagrange relations:

$$\frac{\partial L}{\partial y} - \frac{d}{dt}\frac{\partial L}{\partial \dot{y}} = 0$$

$$\Rightarrow -mg - \frac{d}{dt} m\dot{y} = 0$$

$$\Rightarrow \frac{d}{dt}\frac{dy}{dt} = -g \qquad\qquad y(t) = y_i + v_i t - \tfrac{1}{2} g t^2$$

Modification of Lagrangian due to electric and magnetic fields

For a single particle of charge q using cartesian coordinates and cgs units.

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

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

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

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

Introducing the Hamiltonian --

Lagrangian picture

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

$$L = L\left(\{q_\sigma(t)\},\{\dot{q}_\sigma(t)\},t\right)$$

$$\frac{d}{dt}\frac{\partial L}{\partial \dot{q}_\sigma} - \frac{\partial L}{\partial q_\sigma} = 0$$

$\Rightarrow$ Second order differential equations for $q_\sigma(t)$

Switching variables – Legendre transformation

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

$$H = \sum_\sigma \dot{q}_\sigma p_\sigma - L \qquad \text{where } p_\sigma = \frac{\partial L}{\partial \dot{q}_\sigma}$$

$$dH = \sum_\sigma \left(\dot{q}_\sigma dp_\sigma + p_\sigma d\dot{q}_\sigma - \frac{\partial L}{\partial q_\sigma} dq_\sigma - \frac{\partial L}{\partial \dot{q}_\sigma} d\dot{q}_\sigma \right) - \frac{\partial L}{\partial t} dt$$

Hamiltonian picture – continued

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

$$H = \sum_\sigma \dot{q}_\sigma p_\sigma - L \qquad \text{where} \quad p_\sigma = \frac{\partial L}{\partial \dot{q}_\sigma}$$

$$dH = \sum_\sigma \left(\dot{q}_\sigma dp_\sigma + p_\sigma d\dot{q}_\sigma - \frac{\partial L}{\partial q_\sigma} dq_\sigma - \frac{\partial L}{\partial \dot{q}_\sigma} d\dot{q}_\sigma \right) - \frac{\partial L}{\partial t} dt$$

$$= \sum_\sigma \left(\frac{\partial H}{\partial q_\sigma} dq_\sigma + \frac{\partial H}{\partial p_\sigma} dp_\sigma \right) + \frac{\partial H}{\partial t} dt$$

$$\Rightarrow \dot{q}_\sigma = \frac{\partial H}{\partial p_\sigma} \qquad \frac{\partial L}{\partial q_\sigma} = \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_\sigma} \equiv \dot{p}_\sigma = -\frac{\partial H}{\partial q_\sigma} \qquad \frac{\partial L}{\partial t} = -\frac{\partial H}{\partial t}$$

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 when $\dfrac{dq_\sigma}{dt} = 0$ and/or $\dfrac{dp_\sigma}{dt} = 0$ and/or $\dfrac{dH}{dt} = \dfrac{\partial H}{\partial t} = 0$

we have constant(s) of motion that can be used to help the analysis.