PHY3110 SP23 Notes

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Contents

0 Introduction

Grading: 30% homework, 30% midterm, 40% final.

Textbooks:

- H. Goldstein, C. Poole, J. Safko, Classical Mechanics, 3rd Edition, Pearson.
- J.R. Taylor, Classical Mechanics, University Science Books.
- T.W.B. Kibble, F.H. Berkshire, Classical Mechanics, 5th Edition, Imperial College Press.
- 梁昆淼，力学（下册）理论力学，4^{th} Edition，高等教育出版社.

Classical mechanics describe the motion of macroscopic objects, which are not extremely massive and not extremely fast.

1 Newtonian Mechanics

Vectorial quantities of motion: position $\mathbf{r}$, velocity $\mathbf{v}$, force $\mathbf{F}$, momentum $\mathbf{p} = m\mathbf{v}$, angular momentum $\mathbf{L} = \mathbf{r} \times \mathbf{p}$. Equations of motion are derived from those vector quantities.

Analytical mechanics uses scalar quantities of motion

- Kinetic energy $T = \frac{1}{2}m\mathbf{v}^2$
- Potential energy $V = V(\mathbf{r})$

Equations of motion are derived from those scalar quantities.

1.1 Newton's Laws

Theorem 1.1 (Newton's 2^{nd} law)**.**

$$\mathbf{F} = \frac{\mathrm{d}\mathbf{p}}{\mathrm{d}t} = m\mathbf{a} \tag{1}$$

The formula is valid in an inertial frame.

Angular momentum $\mathbf{L}$ and torque $\mathbf{N}$ are also related

$$\frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}(\mathbf{r} \times \mathbf{p}) = \mathbf{r} \times \mathbf{F} = \mathbf{N} \tag{2}$$

Work done by external forces (note that $\mathrm{d}\mathbf{s} = \mathbf{v}\,\mathrm{d}t$)

$$W_{12} = \int_1^2 \mathbf{F}\,\mathrm{d}\mathbf{s} = \int_1^2 m\frac{\mathrm{d}\mathbf{v}}{\mathrm{d}t}\,\mathrm{d}\mathbf{s} = \int_1^2 m\mathbf{v}\,\mathrm{d}\mathbf{v} = \left.\frac{1}{2}m\mathbf{v}^2\right|_1^2 \tag{3}$$

Define a scalar function $V(\mathbf{r})$, then $\mathbf{F} = -\nabla V(\mathbf{r})$ is a conservative force.

$$\oint \mathbf{F}\,\mathrm{d}\mathbf{s} = 0 \tag{4}$$

Center of mass of the system

$$\mathbf{R} = \frac{\sum_i m_i\mathbf{r}_i}{\sum_i m_i} = \frac{\sum_i m_i\mathbf{r}_i}{M} \tag{5}$$

Total momentum

$$\mathbf{P} = \sum_i m_i \mathbf{p}_i = M\dot{\mathbf{R}} \tag{6}$$

Hence $\mathbf{P}$ is conserved if external force $\mathbf{F}^{(e)}$ is zero.
Total angular momentum

$$\frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t}\sum_i \mathbf{r}_i \times \mathbf{p}_i = \sum_i \mathbf{r}_i \times \left(\mathbf{F}_i^{(e)} + \sum_j \mathbf{F}_{ij}\right) = \sum_i \mathbf{r}_i \times \mathbf{F}_i^{(e)} + \sum_{ij} \mathbf{r}_i \times \mathbf{F}_{ij}$$

Since $\mathbf{r}_{ij}$ parallel to $\mathbf{F}_i j$, then

$$\sum_{ij} \mathbf{r}_i \mathbf{F}_{ij} = \frac{1}{2}\sum_{ij} \mathbf{r}_{ij} \times \mathbf{F}_{ji} = 0 \tag{7}$$

Therefore

$$\frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t} = \mathbf{N}^{(e)} \tag{8}$$

Decomposition of the angular momentum

$$\mathbf{L} = \sum_i \mathbf{r}_i \times \mathbf{p}_i = \sum_i (\mathbf{R} + \mathbf{r}_i) \times m_i(\mathbf{V} + \mathbf{v}'_i) = \sum_i \mathbf{R} \times m_i \mathbf{V} + \sum_i \mathbf{r}'_i \times m_i \mathbf{v}'_i \tag{9}$$

1.2 Constraints

Holonomic constraint

$$f(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N, t) = 0 \tag{10}$$

Example: rigid body

$$(\mathbf{r}_i - \mathbf{r}_j)^2 - c_{ij}^2 = 0 \tag{11}$$

Example: non-sliding cylinder

$$\dot{x} - R\dot{\theta} = 0 \Rightarrow x - R\theta = \text{const}$$

A constraint of the form

$$\sum_i g_i(\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_n)\,\mathrm{d}\mathbf{x}_i = 0 \Rightarrow \mathrm{d}G(\mathbf{x}_1, \dots) = 0 \Rightarrow G(\mathbf{x}_1, \dots) = \text{const} \tag{12}$$

Non-holonomic constraint: cannot be written in the form of holonomic constraint.

1.3 Generalized coordinates

Suppose we have a N-particle system, we will have $3N$ DOFs. With k constraints, we will have $3N - k$ DOFs. Define $q_1, \dots, q_{3N-k}$ generalized coordinates, we have

$$\mathbf{r}_i = \mathbf{r}_i(q_1, \dots, q_{3N-1}, t) \tag{13}$$

2 Lagrange Formalism

2.1 D'Alembert's Principle

Hint from the rigid body: internal forces of constraints do not work.

Virtual displacement: $\delta \mathbf{r}_i$ is consistent with the constraints imposed on the system at a given time

$$\mathbf{r}_i \to \mathbf{r}_i + \delta \mathbf{r}_i \tag{1}$$

Theorem 2.1 (D'Alembert's principle)**.** Consider a system in equilibrium

$$\mathbf{F}_i = 0 \Rightarrow \sum_i \mathbf{F}_i \cdot \delta \mathbf{r}_i = 0 \tag{2}$$

Separate $\mathbf{F}_i = \mathbf{F}_i^{(a)} + \mathbf{f}_i$ where $\mathbf{f}_i$ is the constraint force. Hence

$$\sum_i (\mathbf{F}_i^{(a)} + \mathbf{f}_i) \cdot \delta \mathbf{r}_i = 0 \Rightarrow \sum_i \mathbf{F}_i^{(a)} \cdot \delta \mathbf{r}_i = 0 \tag{3}$$

For a system moving under external forces

$$\mathbf{F}_i - \dot{\mathbf{p}}_i = 0 \Rightarrow \sum_i (\mathbf{F}_i - \dot{\mathbf{p}}_i)\delta \mathbf{r}_i = 0 \Rightarrow \sum_i (\mathbf{F}_i^{(a)} - \dot{\mathbf{p}}_i)\delta \mathbf{r}_i = 0 \tag{4}$$

For holonomic constraints

$$\mathbf{r}_i = \mathbf{r}_i(q_1, \dots, q_n, t), \quad \mathbf{v}_i = \frac{\mathrm{d}\mathbf{r}_i}{\mathrm{d}t} = \frac{\partial \mathbf{r}_i}{\partial t} + \sum_j \frac{\partial \mathbf{r}_i}{\partial q_j}\dot{q}_j, \quad \delta \mathbf{r}_i = \sum_j \frac{\partial \mathbf{r}_i}{\partial q_j}\delta q_j \tag{5}$$

Define generalized force Q_j

$$\sum_i \mathbf{F}_i \delta \mathbf{r}_i = \sum_{ij} \mathbf{F}_i \frac{\partial \mathbf{r}_i}{\partial q_j}\delta q_j = \sum_j Q_j \delta q_j \tag{6}$$

Then

$$\sum_i \dot{\mathbf{p}}_i \cdot \delta \mathbf{r}_i = \sum_{ij} m_i \ddot{\mathbf{r}}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j}\delta q_j = \sum_{ij}\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(m_i \dot{\mathbf{r}}_i \cdot \frac{\partial \mathbf{r}_i}{\partial q_j}\right) - m_i \dot{\mathbf{r}}_i \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathbf{r}_i}{\partial q_j}\right]\delta q_j \tag{7}$$

$$= \sum_j \left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j}\right]\delta q_j = \sum_j Q_j \delta q_j \tag{8}$$

$$\tag{9}$$

where

$$\frac{\partial T}{\partial q_j} = \sum_{ik} \frac{\partial \dot{\mathbf{r}}_k}{\partial q_j}\frac{\partial}{\partial \dot{\mathbf{r}}_k}T = \sum_k m_k \dot{\mathbf{r}}_k \frac{\partial \dot{\mathbf{r}}_k}{\partial q_j} = \sum_k m_k \dot{\mathbf{r}}_k \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathbf{r}_k}{\partial q_j} \tag{10}$$

Hence $\forall j$ we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial T}{\partial \dot{q}_j}\right) - \frac{\partial T}{\partial q_j} - Q_j = 0 \tag{11}$$

Let the potential energy $V = V(\mathbf{r}_i, \dots) = V(q_j, \dots)$, then we have

$$Q_j = \sum_i \mathbf{F}_i \frac{\partial \mathbf{r}_i}{\partial q_j} = \sum_i -\nabla_i V \frac{\partial \mathbf{r}_i}{\partial q_j} = -\frac{\partial V}{\partial q_j} \tag{12}$$

Therefore

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial(T-V)}{\partial\dot{q}_j}\right)-\frac{\partial(T-V)}{\partial q_j}-Q_j=0 \tag{13}$$

Theorem 2.2 (Langrange's equation)**.** Define $L=T-V$, then

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial\dot{q}_j}\right)-\frac{\partial L}{\partial q_j}=0 \tag{14}$$

The choice of Lagrangian is not unique, L' where

$$L'=L+\frac{\mathrm{d}F(q,t)}{\mathrm{d}t} \tag{15}$$

will give the same equations of motion as L.

Example 2.1 (Lagrange's formalism)**.**

1) For a single particle moving under force $\mathbf{F}$

$$L(\mathbf{x},\dot{\mathbf{x}},t)=\frac{1}{2}m\dot{\mathbf{x}}^2+\mathbf{F}\cdot\mathbf{x}$$

2) Motion in a 2D plane using polar coordinates

$$L(r,\theta,\dot{r},\dot{\theta},t)=\frac{1}{2}m(\dot{r}^2+r^2\dot{\theta}^2)+F\cdot\mathbf{r}$$

Generalized forces

$$\begin{aligned}Q_r&=\mathbf{F}\cdot\frac{\partial\mathbf{r}}{\partial r}=\mathbf{F}\cdot\mathbf{e}_r\\ Q_\theta&=\mathbf{F}\cdot\frac{\partial\mathbf{r}}{\partial\theta}=\mathbf{F}\cdot r\mathbf{e}_\theta\end{aligned}$$

where

$$\mathbf{e}_r=\begin{bmatrix}\cos\theta\\ \sin\theta\end{bmatrix}\quad\mathbf{e}_\theta=\begin{bmatrix}-\sin\theta\\ \cos\theta\end{bmatrix}$$

Equations of motion

$$\begin{aligned}m\ddot{r}-mr\dot{\theta}^2&=\mathbf{F}\cdot\mathbf{e}_r\\ mr^2\ddot{\theta}+2mr\dot{r}\dot{\theta}&=r\mathbf{F}_\theta\end{aligned}$$

3) Atwood's machine

$$L=\frac{1}{2}(M_1+M_2)\dot{x}^2+M_1gx+M_2g(l-x)$$

The equation of motion is

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial\dot{x}}-\frac{\partial L}{\partial x}=0\\ \Rightarrow\ &(M_1+M_2)\ddot{x}=(M_1-M_2)g\end{aligned}$$

Suppose we have a potential dependent on velocity (generalized potential) and the generalized force is defined as

$$U=U(q_j,\dot{q}_j),\quad Q_j=-\frac{\partial U}{\partial q_j}+\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial U}{\partial\dot{q}_j} \tag{16}$$

Define $L = T - U$, then we still have

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_j} - \frac{\partial L}{\partial q_j} = 0 \tag{17}$$

Example 2.2 (Lorentz force on a moving charge). The Lorentz force

$$\mathbf{F} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$$

Define the scalar and vector potentials

$$E = -\nabla\phi - \frac{\partial \mathbf{A}}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A}$$

Hence

$$\mathbf{F} = q\left[-\nabla\phi - \frac{\partial \mathbf{A}}{\partial t} + \mathbf{v} \times (\nabla \times \mathbf{A})\right]$$

2.2 Hamilton's principle, variational principle

Configuration space: a space formed by the set of generalized coordinates.

$$(q_1, q_2, \ldots, q_n) \text{ as function of } t \tag{18}$$

Theorem 2.3 (Hamilton's principle). Define the action integral I, where $L = T - V$ or $L = T - U$ (U is the generalized potential)

$$I = \int_{t_1}^{t_2} L \, \mathrm{d}t \tag{19}$$

Then the variation of the action integral equals to zero

$$\delta I = \delta \int_{t_1}^{t_2} L(q_1, \ldots, q_n, \dot{q}_1, \ldots, \dot{q}_n) \, \mathrm{d}t = 0 \tag{20}$$

Add small variation on the path

$$q_i(t, \alpha) = q_i(t) + \alpha\eta(t) \tag{21}$$

where $\eta(t_1) = \eta(t_2) = 0$. Then the action will be the function of α, $I = I(\alpha)$. Hence

$$\delta I = \int_{t_1}^{t_2} \left(\sum_i \frac{\partial L}{\partial q_i}\delta q_i + \frac{\partial L}{\partial \dot{q}_i}\delta \dot{q}_i \right) \mathrm{d}t \tag{22}$$

Change the order of differentiation $\delta \dot{q}_i = \mathrm{d}\delta q_i / \mathrm{d}t$, then

$$\delta I(\alpha) = \int_{t_1}^{t_2} \sum_i \left[\frac{\partial L}{\partial q_i}\delta q_i - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right)\delta q_i \right] \mathrm{d}t + \sum_i \frac{\partial L}{\partial \dot{q}_i}\delta q\Big|_{t_1}^{t_2} \tag{23}$$

$$= \int_{t_1}^{t_2} \sum_i \left[\frac{\partial L}{\partial q_i} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right) \right] \delta q_i \, \mathrm{d}t = 0 \tag{24}$$

$$\Rightarrow \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q_i} = 0 \tag{25}$$

Example 2.3 (Shortest path problem). $y = y(x)$, $\mathrm{d}s = \sqrt{\mathrm{d}x^2 + \mathrm{d}y^2}$, then the action integral (path) is

$$I = \int_1^2 \mathrm{d}s = \int_1^2 \sqrt{1 + \dot{y}^2}\,\mathrm{d}x \tag{26}$$

Apply the Lagrange's equation we get

$$\frac{\mathrm{d}}{\mathrm{d}x}\frac{\mathrm{d}\sqrt{1+\dot{y}^2}}{\mathrm{d}\dot{y}} = 0 \Rightarrow \frac{\mathrm{d}\dot{y}}{\mathrm{d}x} = 0 \Rightarrow y = ax + b \tag{27}$$

Example 2.4 (Solid of revolution). Differential of area $2\pi x\,\mathrm{d}s = 2\pi x\sqrt{1+\dot{y}^2}\,\mathrm{d}x$, then the total area is

$$\int_1^2 2\pi x\sqrt{1+\dot{y}^2}\,\mathrm{d}x \tag{28}$$

Define the Lagrangian $L(x, y, \dot{y}) = 2\pi x\sqrt{1+\dot{y}^2}$, by Lagrange's equation we can get

$$\frac{x\dot{y}}{\sqrt{1+\dot{y}^2}} = \text{const} \Rightarrow y = a\cosh^{-1}\frac{x}{a} + b \tag{29}$$

Example 2.5 (The curve of fastest descent). Question: along which trajectory from point 1 to point 2, the time is shortest? The total time is

$$T = \int_1^2 \frac{\mathrm{d}s}{v} = \int_1^2 \frac{\mathrm{d}s}{\sqrt{2gy}} \tag{30}$$

According to Newton's laws we have $y = gv^2$, then

$$T = \int_1^2 \frac{\sqrt{1+\dot{y}^2}}{\sqrt{2gy}}\,\mathrm{d}x \tag{31}$$

Then we have $L(x, y, \dot{y})$ and we get

$$2y\ddot{y} + 1 + \dot{y}^2 = 0 \tag{32}$$

$$\Rightarrow 2y\dot{y}\ddot{y} + \dot{y} + \dot{y}^3 = \dot{y}(1+\dot{y}^2) + y(2\dot{y}\ddot{y}) = \frac{\mathrm{d}}{\mathrm{d}t}\dot{y}(1+\dot{y}^2) = 0 \tag{33}$$

$$\Rightarrow y(1+\dot{y}^2) = \text{const} \tag{34}$$

which means that $y(1+\dot{y}^2) = \text{const}$. The solution is $x = A(\theta - \sin\theta)$, $y = A(1 - \cos\theta)$.

2.3 Constraint

Holonomic constraints

$$f(q_1, \dots, q_n, t) = 0 \tag{35}$$

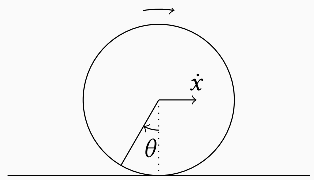
Non-holonomic constraints

$$f(q_1, \dots, q_n; \dot{q}_1, \dots, \dot{q}_n; t) = 0 \tag{36}$$

Sometimes we can convert $f(\dot{q}_i) = 0$ to $f'(q_i) = 0$.

Example 2.6 (Rolling cylinder). Rolling cylinder without sliding has the constraint

$$\dot{x} - R\dot{\theta} = 0 \Rightarrow x - R\theta = \text{const} \tag{37}$$



A commonly encountered type of non-holonomic constraint is linear constraint equations

$$\sum_{k=1}^{n} a_{ik}\frac{\mathrm{d}q_k}{\mathrm{d}t} + a_i t = 0 \tag{38}$$

For the virtual displacement δq_i

$$\sum_{k=1}^{n} a_{ik}\delta q_k = 0 \tag{39}$$

Suppose q_i are not independent, then the Euler-Lagrange's equation could not hold.

$$\int_{t_1}^{t_2}\sum_i\left[\frac{\partial L}{\partial q_i} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_i}\right)\right]\delta q_i\,\mathrm{d}t = 0 \nRightarrow \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}}\right) - \frac{\partial L}{\partial q_i} = 0$$

Include the constraint equation of q_i into the equation

$$\sum_{k=1}^{n} a_{ik}\delta q_k = 0 \Rightarrow \sum_{i=1}^{m}\lambda_i\sum_{k=1}^{n} a_{ik}\delta q_k = 0 \tag{40}$$

Hence

$$\int_{t_1}^{t_2}\sum_{k=1}^{n}\left[\frac{\partial L}{\partial q_k} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_k}\right) + \sum_{i=1}^{m}\lambda_i a_{ik}\right]\delta q_k\,\mathrm{d}t = 0$$

Let $q_1,\dots,q_{n-m}$ be independent generalized coordinate, $q_{n-m+1},\dots,q_n$ dependent generalized coordinates (i.e., they can be expressed by $q_1,\dots,q_{n-m}$). Choose λ_i s.t.

$$\frac{\partial L}{\partial q_k} - \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial L}{\partial \dot{q}_k}\right) + \sum_{i=1}^{m}\lambda_i a_{ik} = 0 \tag{41}$$

$\forall k = n-m+1,\dots,n$. In conclusion, we have $q_1,\dots,q_n,\lambda_1,\dots,\lambda_m$ overall $n+m$ unknowns, and n Lagrange's equations and m constraint equations overall $n+m$ equations.

Remark.

1) It is inconvenient to reduce all q_ks to independent coordinates
2) If we are interested in the constraint forces

$$\sum_{k=1}^{n} a_{ik}\,\mathrm{d}q_k + a_{it}\,\mathrm{d}t = 0$$

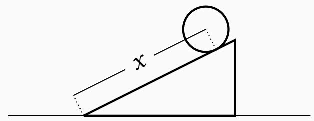
where

$$a_{ik} = \frac{\partial f_i}{\partial q_k},\quad a_{it} = \frac{\partial f_i}{\partial t}$$

Then

$$\mathrm{d}f_i = \frac{\partial f_i}{\partial q_k}\mathrm{d}q_k + \frac{\partial f_i}{\partial t}\mathrm{d}t \Rightarrow \mathrm{d}f_i = 0,\ f_i = \text{const}$$

Example 2.7 (Hoop rooling down an inclined plane).



The constraint equation writes

$$\dot{x} - r\dot{\theta} = 0 \Rightarrow x - r\theta = \text{const}$$

$a_x = 1$, $a_\theta = -r$, $a_t = 0$.
Energy terms are

$$\begin{aligned} T &= T_{\text{COM}} + T_{\text{relative}} = \frac{1}{2}M\dot{x}^2 + \frac{1}{2}M(r\dot{\theta})^2 \\ V &= Mg(l-x)\sin\phi \\ \Rightarrow L &= \frac{1}{2}M\dot{x}^2 + \frac{1}{2}M(r\dot{\theta})^2 - Mg(l-x)\sin\phi \end{aligned}$$

Then we can write the Lagrange's equation with Lagrange's multipliers

$$\begin{aligned} \frac{\partial L}{\partial x} - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} + a_x\lambda = 0 \\ \Rightarrow Mg\sin\phi - M\ddot{x} + \lambda = 0 \\ -Mr^2\ddot{\theta} - \lambda r = 0 \\ \dot{x} = r\dot{\theta} \Rightarrow \ddot{x} = r\ddot{\theta} \end{aligned}$$

we can get $M\ddot{x} = Mr\ddot{\theta} = -\lambda$ and $\ddot{x} = (g\sin\phi)/2$. Note that λ is the constraint force (in this case λ is the frictional force).

Theorem 2.4 (Universal test for holonomic constraints). Let the constraint equation be

$$\sum_j A_j \,\mathrm{d}u_j = 0 \tag{42}$$

Then we can test the equation where

$$A_\gamma\left(\frac{\partial A_\beta}{\partial u_\alpha} - \frac{\partial A_\alpha}{\partial u_\beta}\right) + A_\beta\left(\frac{\partial A_\alpha}{\partial u_\gamma} - \frac{\partial A_\gamma}{\partial u_\alpha}\right) + A_\alpha\left(\frac{\partial A_\gamma}{\partial u_\beta} - \frac{\partial A_\beta}{\partial u_\gamma}\right) = 0 \tag{43}$$

2.4 Lagrangian for Lorentz force

The Lorentz force is given by

$$\mathbf{F} = q[\mathbf{E} + \mathbf{v} \times \mathbf{B}] \tag{44}$$

Where

$$\mathbf{E} = -\nabla\phi - \frac{\partial A}{\partial t}, \quad \mathbf{B} = \nabla \times \mathbf{A} \tag{45}$$

Hence, by defining the Lagrangian

$$L = \frac{1}{2}m\mathbf{v}^2 - q\phi + q\mathbf{A}\cdot\mathbf{v} \tag{46}$$

Applying the Lagrange's equation we can get the EOM (eq. 44). Take x as an example

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{x}} = \frac{\mathrm{d}}{\mathrm{d}t}(m\dot{x} + qA_x) = m\ddot{x} + q\frac{\partial A_x}{\partial t} + \mathbf{v}\cdot\nabla A_x \tag{47}$$

2.5 Conservation & symmetry of the system

Definition 2.1 (Cylic coordinate). The generalized coordinate q_i is cyclic (ignorable) if

$$\frac{\partial L}{\partial q_i} = 0 \tag{48}$$

It implies the generalized momentum p_i is conserved.

Rotational symmetry. Let q_j be one of the rotational angle of spacial coordinate $\mathbf{r}_i$. Hence

$$\mathrm{d}\mathbf{r}_i = \mathbf{n}_j \times \mathbf{r}_i \,\mathrm{d}q_j \Rightarrow \frac{\partial \mathbf{r}_i}{\partial q_j} = \mathbf{n}_j \times \mathbf{r}_i \,\mathrm{d}q_j \tag{49}$$

where $\mathbf{n}_j$ is the normal vector of the rotation axis of q_j. Hence the generalized force of q_j writes

$$Q_{q_j} = -\frac{\partial V}{\partial q_j} = -\sum_k \frac{\partial V}{\partial \mathbf{r}_k}\frac{\partial \mathbf{r}_k}{\partial q_j} = -\frac{\partial V}{\partial \mathbf{r}_i}\frac{\partial \mathbf{r}_i}{\partial q_j} = \mathbf{F}_i \cdot (\mathbf{n}_j \times \mathbf{r}_i) = \mathbf{n}_j \cdot (\mathbf{r}_i \times \mathbf{F}_i) = \mathbf{n}_j \cdot \mathbf{N}_i \tag{50}$$

where $\mathbf{N}_i$ stands for the torque on the i^{th} particle. The generalized momentum of q_j writes

$$p_{q_j} = \frac{\partial T}{\partial \dot{q}_j} = \sum_k \frac{\partial T}{\partial \dot{\mathbf{r}}_k}\frac{\partial \mathbf{r}_i}{\partial q_j} = \sum_k m_k \dot{\mathbf{r}}_k \cdot \frac{\partial \dot{\mathbf{r}}_k}{\partial \dot{q}_j} = m_i \dot{\mathbf{r}}_i \cdot (\mathbf{n}_j \times \mathbf{r}_i) = \mathbf{n}_j \times (\mathbf{r}_i \times m_i \dot{\mathbf{r}}_i) = \mathbf{r}_j \times \mathbf{L}_i \tag{51}$$

where $\mathbf{L}_i$ stands for the angular momentum of the i^{th} particle. Hence, the rotational invariance implies the conservation of angular momentum.

Time translation

$$\begin{aligned}
\frac{\mathrm{d}}{\mathrm{d}t}L &= \sum_i \frac{\partial L}{\partial q_i}\dot{q}_i + \frac{\partial L}{\partial \dot{q}_i}\ddot{q}_i + \frac{\partial L}{\partial t} &(52)\\
&= \sum_i \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i + \frac{\partial L}{\partial \dot{q}_i}\ddot{q}_i + \frac{\partial L}{\partial t} &(53)\\
&= \frac{\mathrm{d}}{\mathrm{d}t}\sum_i \left(\frac{\partial L}{\partial \dot{q}_i}\dot{q}_i\right) + \frac{\partial L}{\partial t} &(54)\\
\Rightarrow \frac{\partial L}{\partial t} &+ \frac{\mathrm{d}}{\mathrm{d}t}\underbrace{\left(\sum \frac{\partial L}{\partial \dot{q}_i} q_i - L\right)}_{H} = 0 &(55)
\end{aligned}$$

Note that

$$\sum_i \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i = 2T \tag{56}$$

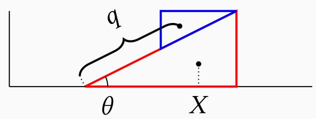
Proof. Suppose r_i does not have explicit time dependence ($\partial r_i/\partial t = 0$)

$$\begin{aligned}
T &= \sum_i \frac{1}{2}m_i \dot{r}_i^2 = \sum_i \frac{1}{2}m_i \left(\sum_j \frac{\partial r_i}{\partial q_j}\dot{q}_j + \frac{\partial r_i}{\partial t}\right)^2\\
&= \sum_{ijk} \frac{1}{2}m_i \frac{\partial r_i}{\partial q_j}\frac{\partial r_i}{\partial q_k}\dot{q}_j\dot{q}_k\\
\Rightarrow \sum_i \frac{\partial L}{\partial \dot{q}_i}\dot{q}_i &= \sum_i \dot{q}_i \sum_{jk} m_k \frac{\partial r_k}{\partial q_i}\frac{\partial r_k}{\partial q_j}\dot{q}_j = \sum_{ijk} m_k \frac{\partial r_k}{\partial q_i}\frac{\partial r_k}{\partial q_j}\dot{q}_i\dot{q}_j = 2T
\end{aligned}$$

□

Hence we can define Hamiltonian $H = T + V$ which stands for the total energy, and H conserved if L doesn't depend on time explicitly.

Example 2.8 (Two blocks). Let M be the mass of the big block, m be the mass of the small block. Define two generalized coordinates: X stand for the position of COM of the big block, q stand for the position of COM of the small block (sloped).



Hence we can easily define the Lagrangian

$$L = \frac{1}{2}M\dot{X}^2 + \frac{1}{2}m[(\dot{X} + \dot{q}\cos\theta)^2 + \dot{q}^2\sin^2\theta] - mgq\sin\theta$$

There is no X dependence on the system, hence X is a cyclic coordinate.

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{X}} &= \frac{\mathrm{d}}{\mathrm{d}t}M\dot{X} + m(\dot{X} + \dot{q}\cos\theta) = 0\\ \Rightarrow& M\dot{X}m(\dot{X} + \dot{q}\cos\theta) = p_X = \mathrm{const}\end{aligned}$$

3 The Central Force Problem

3.1 Reduction to the equivalent one-body problem

For the two-body problem, we have two choices of generalized coordinate

(a) $\mathbf{r}_1, \mathbf{r}_2$ stand for spacial coordinates of two masses

(b) $\mathbf{R}$ spacial coordinate of the COM, $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$

Hence, we can rewrite the kinetic energy in terms of $\mathbf{R}$ and $\mathbf{r}$

$$
\begin{aligned}
T &= \frac{1}{2}m_1\dot{\mathbf{r}}_1^2 + \frac{1}{2}m_2\dot{\mathbf{r}}_2^2 && (1)\\
&= \frac{1}{2}m_1\left(\dot{\mathbf{R}} + \frac{m_2}{m_1+m_2}\dot{\mathbf{r}}\right)^2 + \frac{1}{2}m_2\left(\dot{\mathbf{R}} - \frac{m_1}{m_1+m_2}\dot{\mathbf{r}}\right)^2 && (2)\\
&= \frac{1}{2}(m_1+m_2)\dot{\mathbf{R}}^2 + \frac{m_1 m_2}{m_1+m_2}\dot{\mathbf{r}}^2 = \frac{1}{2}M\dot{\mathbf{R}}^2 + \frac{1}{2}\mu\dot{\mathbf{r}}^2 && (3)
\end{aligned}
$$

Hence we can write the Lagrangian

$$
L = \frac{1}{2}M\dot{\mathbf{R}}^2 + \frac{1}{2}\mu\dot{\mathbf{r}}^2 - V \tag{4}
$$

Suppose $V = V(\mathbf{r})$, then $\mathbf{R}$ is a cyclic coordinate, We have $\dot{\mathbf{R}} = \text{const}$, and we can drop $\dot{\mathbf{R}}$ terms in L. Moreover, if $V = V(\|\mathbf{r}\|)$, the total angular momentum is conserved.

Use r, θ as generalized coordinates, we have

$$
L = \frac{1}{2}\mu(\dot{r}^2 + r^2\dot{\theta}^2) - V(r) \tag{5}
$$

The Lagrange's equation wrt r writes

$$
\mu\ddot{r} - \mu r\dot{\theta}^2 + \frac{\partial V}{\partial r} = 0 \tag{6}
$$

Easy to find that θ is cyclic, hence

$$
\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial\dot{\theta}} = \frac{\mathrm{d}}{\mathrm{d}t}\mu r^2\dot{\theta} = 0 \Rightarrow p_\theta = \mu r^2\dot{\theta} = l = \text{const} \tag{7}
$$

Theorem 3.1 (Kepler's 2nd law)**.** Radius vector sweeps out equal areas in equal time.

Substitute $\mu r\dot{\theta}^2$ term by L, we have

$$
\begin{aligned}
\mu\ddot{r} - \frac{l^2}{\mu r^3} + \frac{\partial V}{\partial r} &= 0 && (8)\\
\Rightarrow \mu\ddot{r} &= -\frac{\partial}{\partial r}(V + \frac{l^2}{2\mu r^2}) && (9)\\
\mu\ddot{r}\dot{r} &= -\frac{\partial}{\partial r}\dot{r}(V + \frac{l^2}{2\mu r^2}) && (10)\\
\Rightarrow \frac{\mathrm{d}}{\mathrm{d}t}(\frac{1}{2}\mu\dot{r}^2 + V + \frac{l^2}{2\mu r^2}) &= \frac{\mathrm{d}}{\mathrm{d}t}E = 0 && (11)
\end{aligned}
$$

Hence we can get the expression of $\dot{r}$ and a differential equation

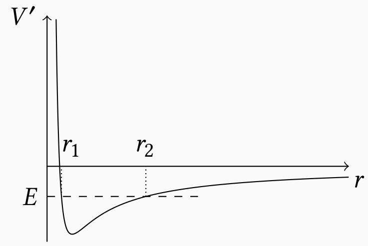
$$
\dot{r} = \sqrt{\frac{2}{\mu}(E - V - \frac{l^2}{2\mu r^2})} \tag{12}
$$

Define the new effective force $f'(r)$ with an effective potential $V' = V + l^2/2\mu r^2$, we have

$$
\mu\ddot{r} = -\frac{\partial V}{\partial r} + \frac{l^2}{\mu r^3} = f'(r), \quad E = \frac{1}{2}\mu\dot{r}^2 + V' = \text{const} \tag{13}
$$

Example 3.1 (Gravitational force). Suppose we have $f(r) = -kr^{-2}$ and $V = -kr^{-1}$, then

$$V' = -\frac{k}{r} + \frac{l^2}{2\mu r^2}$$



1) $E = E_1 \geq 0$, the motion has a lower bound, $r \geq r_1$.
2) $V_{\text{min}} < E_2 < 0$, the motion has lower and upper bound, $r_1 \leq r \leq r_2$.
3) $E_3 = V_{\text{min}}$, the motion will shrink to a single circle $r_1 = r_2 = \text{const}$, hence it is a circular motion. In this case, the gravitational force is equal to the centrifugal force

$$\mu\ddot{r} = f(r) + \frac{l^2}{\mu r^3} = f(r) + \mu r\dot{\theta}^2 = 0 \Rightarrow f(r) = -\mu r\dot{\theta}^2$$

Remark. Let the potential be $V = -kr^{-\alpha}$, then the motion cannot have periodic behavior if $\alpha > 2$.

Example 3.2 (Harmonic oscillator). $V = kr^2/2$, we have

$$V' = \frac{1}{2}kr^2 + \frac{l^2}{2\mu r^2}$$

Theorem 3.2 (Conditions for closed orbitals, Bertrand's theorem). Stable orbitals require

$$\left.\frac{\partial^2 V'}{\partial r^2}\right|_{r=r_0} = \left.-\frac{\partial f}{\partial r} + \frac{3l^2}{mr^4}\right|_{r=r_0} > 0 \Rightarrow \left.\frac{\partial f}{\partial r}\right|_{r=r_0} < -\frac{3f(r_0)}{r_0} \tag{14}$$

Let $f = -kr^n$, then we have

$$-knr^{n-1} < 3kr^{n-1} \Rightarrow n > -3 \tag{15}$$

For a small perturbation from the minimum, we can write the effective potential as Taylor expansion

$$V'(r) = V'(r_0) + \left.\frac{\partial V'}{\partial r}\right|_{r=r_0}(r - r_0) + \frac{1}{2}\left.\frac{\partial^2 V'}{\partial r^2}\right|_{r=r_0}(r - r_0)^2 + \cdots \tag{16}$$

$$= V'(r_0) + \frac{1}{2}\left.\frac{\partial^2 V'}{\partial r^2}\right|_{r=r_0}(r - r_0)^2 + O(|r - r_0|^3) \tag{17}$$

Hence the EOM becomes

$$m\ddot{r} = -\frac{\partial V'}{\partial r} = -\left.\frac{\partial^2 V'}{\partial r^2}\right|_{r=r_0}(r - r_0) \tag{18}$$

$$\dot{\theta} = \frac{l}{mr^2} \tag{19}$$

The solution taks the form

$$u = u_0 + a\cos\beta\theta,\ u = \frac{1}{r},\ \beta^2 = \left.\frac{r}{f}\frac{\partial f}{\partial r} + 3\right|_{r=r_0} \tag{20}$$

For finite perturbation, the orbit can be a closed only if $\beta^2 = 1$ or 4. Then there are only two types of central-force scalar problem with the property that all bound orbitals are closed orbitals.

$$\left.\frac{r}{f}\frac{\partial f}{\partial r}\right|_{r=r_0} = \pm 2 \Rightarrow f = -kr^{-2} \text{ or } -kr \tag{21}$$

check the theorem on other books

3.2 Virial theorem

Consider a multi-particle system $1 \le i \le N$.

$$\dot{\mathbf{p}}_i = \mathbf{F}_i \tag{22}$$

Define new function

$$G = \sum_i \mathbf{p}_i \cdot \mathbf{r}_i \tag{23}$$

Then the time derivative of G writes

$$\frac{\mathrm{d}}{\mathrm{d}t}G = \sum_i m_i \dot{\mathbf{r}}_i^2 + \sum_i \mathbf{F}_i \cdot \mathbf{r}_i \tag{24}$$

Hence the time average of $\mathrm{d}G/\,\mathrm{d}t$ is

$$\frac{1}{\tau}\int_0^\tau \frac{\mathrm{d}}{\mathrm{d}t}G\,\mathrm{d}t = 2\overline{T} + \overline{\sum_i \mathbf{F}_i \cdot \mathbf{r}_i} = \frac{1}{\tau}[G(\tau) - G(0)] \tag{25}$$

The time average equals to 0 if τ is the period of the periodic motion; even for non-periodic motion, if $\tau \to \infty$, the average will approach 0. Hence

$$2\overline{T} + \overline{\sum_i \mathbf{F}_i \cdot \mathbf{r}_i} = 0 \Rightarrow \overline{T} = -\frac{1}{2}\underbrace{\overline{\sum_i \mathbf{F}_i \cdot \mathbf{r}_i}}_{\text{virial of Clausius}} \tag{26}$$

Example 3.3 (Ideal gas)**.** Temperature $T \propto T_i$ kinetic energy of i^{th} particle.

$$T_i = \frac{3}{2}k_B T \tag{27}$$

Hence the time average of total kinetic energy is

$$\overline{\sum_i T_i} = \frac{3}{2}Nk_B T \tag{28}$$

The virial could be written as

$$\overline{\sum_i \mathbf{F}_i \cdot \mathbf{r}_i} = \int \mathrm{d}\mathbf{F} \cdot \mathbf{r} \tag{29}$$

Note that

$$\mathrm{d}\mathbf{F} = -p\,\mathrm{d}A\mathbf{n}$$

Applying Gauss's law we have

$$\overline{\sum_i \mathbf{F}_i \cdot \mathbf{r}_i} = -\int p\,\mathrm{d}A\;\mathbf{n} \cdot \mathbf{r} = -\int p\,\mathrm{d}V\;(\nabla \mathbf{r}) = -3pV \tag{30}$$

Hence by the equation we get $pV = nk_B T$.

Example 3.4 (Gravational force). Since $\mathbf{F}_i = -\nabla_i V$, given $V_i = ar_i^{n+1}$, we have

$$\overline{T} = \frac{1}{2}\overline{\sum_i \nabla_i V \cdot \mathbf{r}_i} = \frac{n+1}{2}\overline{\sum_i ar_i^{n+1}} = \frac{n+1}{2}\overline{V} \tag{31}$$

This theorem is particularly important when the potential energy is a homogeneous function of the coordinates, i.e.

$$U(\alpha\mathbf{r}_1, \dots, \alpha\mathbf{r}_n) = \alpha^k U(\mathbf{r}_1, \dots, \mathbf{r}_n) \tag{32}$$

Note that

$$\frac{\mathrm{d}U}{\mathrm{d}\alpha} = \sum_a \frac{\partial \alpha\mathbf{r}_a}{\partial\alpha} \cdot \frac{\partial U}{\partial \alpha\mathbf{r}_a} = \sum_a \frac{\mathbf{r}_a}{\alpha} \cdot \frac{\partial U}{\partial \mathbf{r}_a} = k\alpha^{k-1}U \tag{33}$$

Then the equation 26 becomes

$$2\overline{T} = k\overline{U} \tag{34}$$

Equivalently

$$\overline{U} = \frac{2E}{k+2}, \ \overline{T} = \frac{kE}{k+2} \tag{35}$$

3.3 Inverse-square force

Consider $f = -k/r^2$, $V = -k/r$, then we have EOM

$$\dot{r} = \left[\frac{2}{m}\left(E + \frac{k}{r} - \frac{l^2}{2mr^2}\right)\right]^{1/2} \Rightarrow \theta = \theta_0 + \int_{r_0}^{r_1} \frac{\mathrm{d}r}{r^2\left(\frac{2mE}{l^2} - \frac{2mV}{l^2} - \frac{1}{r^2}\right)^{1/2}} \tag{36}$$

Define $u = 1/r$, let $\theta_0 = 0$, then

$$\theta = \theta_0 - \int_{u_0}^{u_1} \frac{\mathrm{d}u}{\left(\frac{2mE}{l^2} + \frac{2mku}{l^2} - u^2\right)^{1/2}} \tag{37}$$

$$\Rightarrow \theta = -\arccos\frac{\frac{l^2u}{mk} - 1}{\sqrt{1 + \frac{2El^2}{mk^2}}}, \ r = \frac{\frac{l^2}{mk}}{1 + \sqrt{1 + \frac{2El^2}{mk^2}}\cos\theta} = \frac{r_0}{1 + \epsilon\cos\theta} \tag{38}$$

ϵ is called the eccentricity.

ϵ	Energy	Orbit
$\epsilon > 1$	$E > 0$	Hyperbola
$\epsilon = 1$	$E = 0$	Parabola
$0 < \epsilon < 1$	$E < 0$	Ellipse
$\epsilon = 0$	$E < 0$	Circle

The major semi-axis a and minor semi-axis b are given by

$$a = \frac{r_0}{1-\epsilon^2} = -\frac{k}{2E}, \ b = a\sqrt{1-\epsilon^2} = \frac{k}{\sqrt{-2mE}} \tag{39}$$

Since $mr^2\dot{\theta} = l$, then

$$\int_0^T \mathrm{d}A = \frac{1}{2}\int_0^T r^2\dot{\theta}\,\mathrm{d}t = \frac{1}{2}\int_0^T \frac{l}{m}\theta\,\mathrm{d}t = \frac{l}{2m}T = \pi ab \Rightarrow T = 2\pi a^{3/2}\sqrt{\frac{m}{k}} \tag{40}$$

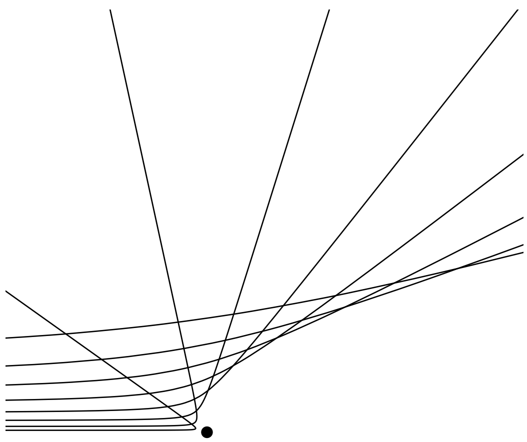
Alternatively

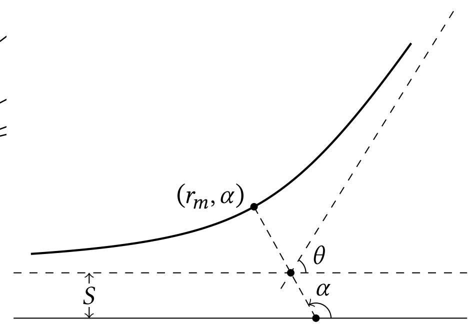
$$\int \mathrm{d}t = \int \frac{\mathrm{d}r}{\sqrt{\frac{2}{m}\left(E - V - \frac{l^2}{2mr^2}\right)}} = \sqrt{\frac{ma}{k}} \int_{r_0}^{r_1} \frac{r\,\mathrm{d}r}{\sqrt{-r^2 + 2ar - b^2}} = \sqrt{\frac{ma}{k}} \int_{r_0}^{r_1} \frac{r\,\mathrm{d}r}{\sqrt{-(r-a)^2 + a^2\epsilon^2}} \tag{41}$$

Let $r - a = -a\epsilon\cos\zeta$, hence

$$t = \sqrt{\frac{ma}{k}} \int \frac{(a - a\epsilon\cos\zeta)a\epsilon\sin\zeta\,\mathrm{d}\zeta}{\sqrt{a\epsilon^2(1-\cos^2\zeta)}} = \sqrt{\frac{ma}{k}} \int (a - a\epsilon\cos\zeta)\,\mathrm{d}\zeta = \sqrt{\frac{ma^3}{k}}(\zeta - \epsilon\sin\zeta) + C \tag{42}$$

3.4 Scattering





Question: how many particles will be scattered in the given solid angle region (scattering cross section). Let $V \sim 1/r$, $f \sim 1/r^2$. Define the intensity of incident beam I

$$I = \#\text{ of particles crossing a unit area perpendicular to the beam in unit time}$$

The the number of particles scattered into $\mathrm{d}\Omega$ could be expressed as

$$\mathrm{d}N = \sigma I\,\mathrm{d}\Omega,\ \sigma = \frac{\mathrm{d}N}{I\,\mathrm{d}\Omega} \tag{43}$$

where σ is called differential cross section, which has the unit of area.

Particles in $[S, S + \mathrm{d}S]$ would be scattered into $[\Omega, \Omega + \mathrm{d}\Omega]$, since $\mathrm{d}\Omega = 2\pi\sin\theta\,\mathrm{d}\theta$

$$2\pi IS|\,\mathrm{d}S| = \sigma I\,\mathrm{d}\Omega = 2\pi\sigma I\sin\theta|\,\mathrm{d}\theta| \Rightarrow \sigma = \frac{S|\,\mathrm{d}S|}{\sin\theta|\,\mathrm{d}\theta|} \tag{44}$$

The angular momentum of the incoming particles (wrt. to force center) is

$$l = mv_0S = S\sqrt{2mE} \tag{45}$$

From the equation derived from central force problem

$$\alpha = \int \frac{\mathrm{d}r}{r^2\sqrt{\frac{2mE}{l^2} - \frac{rmV}{l^2} - \frac{1}{r^2}}} \tag{46}$$

$$= \pi + \int_{-\infty}^{r_m} \frac{\mathrm{d}r}{r^2\sqrt{\frac{2mE}{l^2} - \frac{rmV}{l^2} - \frac{1}{r^2}}} \tag{47}$$

Let $r_m \equiv r_{\text{min}}$ is the closest distance. Define ψ where

$$\alpha = \pi + \int_{-\infty}^{r_m} \frac{\mathrm{d}r}{r^2\sqrt{\frac{2mE}{l^2} - \frac{rmV}{l^2} - \frac{1}{r^2}}} = \pi - \psi \tag{48}$$

Hence $\theta = \pi - 2\psi$. Change the variable $u = 1/r$, then

$$\psi = \int_0^{u_m = 1/r_m} \frac{S\,\mathrm{d}u}{\sqrt{1 - \frac{V}{E} - S^2u^2}} \tag{49}$$

Also note that

$$\sin\frac{\theta}{2} = \sin\frac{\pi - 2\psi}{2} = \cos\psi = \frac{1}{\epsilon} \tag{50}$$

Example 3.5 (Coulomb interaction)**.** Let

$$f = \frac{ZZ'e^2}{r^2},\ V = \frac{ZZ'e^2}{r},\ r = \frac{r_0}{1 + \epsilon\cos(\alpha - \alpha')} \tag{51}$$

choose $\alpha' = \pi$. One can derive that

$$\epsilon = \sqrt{1 + \frac{2El^2}{m(ZZ'e^2)^2}} = \sqrt{1 + \left(\frac{2ES}{ZZ'e^2}\right)^2} \tag{52}$$

Using the trigonometric relationship between θ and ϵ, we have

$$S = \frac{ZZ'e^2}{2E}\cot\frac{\theta}{2},\ \left|\frac{\mathrm{d}S}{\mathrm{d}\theta}\right| = \frac{ZZ'e^2}{4E}\frac{1}{\sin^2\frac{\theta}{2}} \tag{53}$$

$$\Rightarrow \epsilon(\theta) = \left(\frac{ZZ'e^2}{4E}\right)^2 \frac{1}{\sin^4\frac{\theta}{2}} \tag{54}$$

check if $\alpha' = \pi$ or $\alpha' = \alpha_m$

4 Rigid Body

4.1 Coordinates of rigid body

A rigid body is a system of point masses satisfying the constraint that distance between any two points is a constant (r_{ij} = const for all i, j). Let $\mathbf{r}_i$, $\mathbf{r}_j$, and $\mathbf{r}_k$ be three points in the rigid body. Let $\mathbf{r}_i$ has 3 DOFs, since $r_i j$ is a constant, $\mathbf{r}_j$ has two DOFs. Hence, $\mathbf{r}_k$ only have 1 DOFs. The system has $3 + 2 + 1 = 6$ DOFs.

Or, alternatively, a rigid body has 3 coordinates for the origin of the coordinate system fixed on the rigid body, and 3 angular variables to specify the orientation of the rotated coordinate system.

4.2 Orthogonal transformations

Consider an orthogonal transformation $\mathbf{x} \mapsto \mathbf{x}'$

$$x_1' = a_{11}x_1 + a_{12}x_2 + a_{13}x_3 \tag{1}$$
$$x_2' = a_{21}x_1 + a_{22}x_2 + a_{23}x_3 \tag{2}$$
$$x_3' = a_{31}x_1 + a_{32}x_2 + a_{33}x_3 \tag{3}$$

Let $\mathbf{x}^2 = \mathbf{x}'^2$, we have

$$\mathbf{x}^2 = x_i x_i = x_i' x_i' = a_{ij}x_j a_{ik}x_k = \delta_{jk}x_j x_k = x_j x_j \Rightarrow a_{ij}a_{ik} = \delta_{jk} \tag{4}$$

This equation implies the orthogonal transformations have three DOFs.

Different views on rotational transformation

1. Passive view the coordinate system is transformed
2. Active view: the vector is transformed

Consider two rotational matrix A and B, let $C = AB$, then

$$C_{ij}C_{ik} = A_{im}B_{mj}A_{in}B_{nk} = A_{im}A_{in}B_{mk}B_{nk} = \delta_{nm}B_{mj}B_{nk} = B_{nj}B_{nk} = \delta_{jk} \tag{5}$$

Non-commutative $AB \neq BA$.

Define the inverse transformation

$$x_i = a'_{ij}x'_j = a'_{ij}a_{jk}x_k \Rightarrow a'_{ij}a_{jk} = \delta_{ik} \tag{6}$$

Note that

$$\left.\begin{aligned} \underbrace{a_{im}a_{ij}}_{i} a'_{jk} &= \delta_{mk}a'_{jk} = a'_{mk} \\ a_{im}\underbrace{a_{ij}a'_{jk}}_{j} &= a_{im}\delta_{ik} = a_{km} \end{aligned}\right\} \Rightarrow a_{km} = a'_{mk} \tag{7}$$

4.3 Euler angles

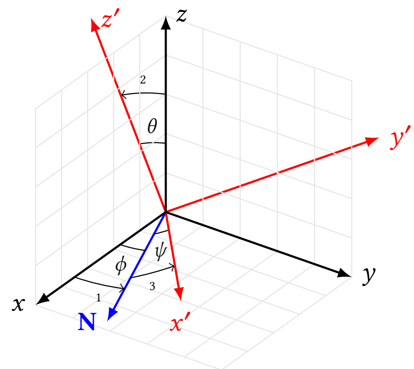
A convenient choice of angle variables: Euler angles. Steps:

1. Rotate around z axis by an angle ϕ, rotational matrix D
2. Rotate around ξ axis by an angle θ, rotational matrix C
3. Rotate around ξ' axis by an angle ψ, rotational matrix B

We can always write any rotational matrix A as $A = BCD$ Note that all rotations are rotations of **coordinate system**, which means, A is a change-of-basis matrix.

$$A = \begin{bmatrix} \cos\psi & \sin\psi & 0 \\ -\sin\psi & \cos\psi & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & \sin\theta \\ 0 & -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\phi & \sin\phi & 0 \\ -\sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{8}$$

$$= \begin{bmatrix} \cos\phi\cos\psi - \cos\theta\sin\phi\sin\psi & \cos\psi\sin\phi + \cos\theta\cos\phi\sin\psi & \sin\theta\sin\psi \\ -\cos\theta\cos\psi\sin\phi - \cos\phi\sin\psi & \cos\theta\cos\phi\cos\psi - \sin\phi\sin\psi & \cos\psi\sin\theta \\ \sin\theta\sin\phi & -\cos\phi\sin\theta & \cos\theta \end{bmatrix} \tag{9}$$



Theorem 4.1 (Euler's theorem)**.** The general displacement of a rigid body with one point fixed is a rotation around some axis $\mathbf{R}$. Then

$$\mathbf{R}' = A\mathbf{R} = \mathbf{R} \Rightarrow (A - I)\mathbf{R} = 0, \ \det(A - I) = 0 \tag{10}$$

Infinitesimal rotation transformation

$$\mathbf{x}' = A\mathbf{x} = (1+\epsilon)\mathbf{x} \Rightarrow x_i' = x_i + \epsilon_{ij}x_j = (\delta_{ij} + \epsilon_{ij})x_j \tag{11}$$

Hence

$$(\delta_{ki} + \epsilon_{ki}')x_i' = (\delta_{ki} + \epsilon_{ki}')(\delta_{ij} + \epsilon_{ij})x_j = (\delta_{kj} + \epsilon_{kj}' + \epsilon_{kj} + \epsilon_{ki}'\epsilon_{ij})x_j = x_k \tag{12}$$

Ignoring $\epsilon_{ki}'\epsilon_{ij}$ term, we have $\epsilon_{kj}' = \epsilon_{jk}^T = -\epsilon_{kj}$, given that ϵ is an antisymmetric matrix. Let

$$\epsilon = \begin{bmatrix} 0 & -d\Omega_3 & \mathrm{d}\Omega_2 \\ \mathrm{d}\Omega_3 & 0 & -\mathrm{d}\Omega_1 \\ -\mathrm{d}\Omega_2 & \mathrm{d}\Omega_1 & 0 \end{bmatrix}, \ \boldsymbol{\Omega} = \begin{bmatrix} \Omega_1 \\ \Omega_2 \\ \Omega_3 \end{bmatrix} \tag{13}$$

Then

$$\mathrm{d}\mathbf{x} = \epsilon\mathbf{x} = \mathrm{d}\boldsymbol{\Omega} \times \mathbf{x} \tag{14}$$

4.4 Rate of change of a vector

Let $\mathbf{R}$ be one point inside the rigid body, then the motion can be decomposed into rotational motion of the body coordinate and the translational motion of the body

$$\left(\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t}\right)_{\text{space}} = \left(\frac{\mathrm{d}\mathbf{R}}{\mathrm{d}t}\right)_{\text{body}} + \frac{\mathrm{d}\Omega}{\mathrm{d}t} \times \mathbf{R} \tag{15}$$

$$\Rightarrow \mathbf{V}_{\text{space}} = \mathbf{V}_{\text{body}} + \boldsymbol{\omega} \times \mathbf{R} \tag{16}$$

Decompose $\boldsymbol{\omega}$ into unit vectors corresponds to Euler angles and the body coordinate

$$\boldsymbol{\omega} = \dot{\phi}e_\phi + \dot{\theta}e_\theta + \dot{\psi}e_\psi = \omega_{x'}\mathbf{i}' + \omega_{y'}\mathbf{j}' + \omega_{z'}\mathbf{k}' \tag{17}$$

From the figure we can find that

$$e_\phi = \mathbf{k} = \sin\theta\sin\psi\mathbf{i}' + \sin\theta\cos\psi\mathbf{j}' + \cos\theta\mathbf{k}' \tag{18}$$

$$e_\theta = \cos\psi\mathbf{i}' - \sin\psi\mathbf{j}' \tag{19}$$

$$e_\psi = \mathbf{k}' \tag{20}$$

Hence

$$\begin{aligned} \omega_{x'} &= \dot{\phi}\sin\theta\sin\psi + \dot{\theta}\cos\psi && (21)\\ \omega_{y'} &= \dot{\phi}\sin\theta\cos\psi - \dot{\theta}\sin\psi && (22)\\ \omega_{z'} &= \dot{\psi} + \dot{\phi}\cos\theta && (23) \end{aligned}$$

4.5 The Coriolis effect

From equation 16 we have

$$\begin{aligned} \mathbf{a}_{\text{space}} &= \mathbf{a}_{\text{body}} + \boldsymbol{\omega}\times\mathbf{V} && (24)\\ \Rightarrow m\mathbf{a}_{\text{body}} &= \mathbf{F} - 2m\omega\times\mathbf{V}_{\text{body}} - m\omega\times(\boldsymbol{\omega}\times\mathbf{R}) && (25) \end{aligned}$$

The term $-2m\omega\times\mathbf{V}_{\text{body}}$ is the Coriolis force.

Remark. Since $\mathbf{V}_{\text{body}}$ is also rotating around $\boldsymbol{\omega}$, we have

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{V}_{\text{body}} = \mathbf{a}_{\text{body}} + \boldsymbol{\omega}\times\mathbf{V}_{\text{body}} \tag{26}$$

Additional notes on transformation of basis

Remark. One can check Arnold's CM book for comprehensive mathematical formulation for spacial transformation.

5 EOM of rigid body

5.1 Angular momentum and kinetic energy

It is often convenient to choose the COM of the rigid body as the origin of the body system. Suppose the motion only involves rotation, the angular momentum is

$$\mathbf{L} = \sum_i m_i(\mathbf{r}_i \times \mathbf{v}_i) = \sum_i m_i[\mathbf{r}_i \times (\boldsymbol{\omega} \times \mathbf{r}_i)] = \sum_i m_i[\mathbf{r}_i^2\boldsymbol{\omega} - \mathbf{r_i}(\mathbf{r}_i \cdot \boldsymbol{\omega})] \tag{1}$$

Consider the components of the equation

$$L_x = \sum_i m_i[\omega_x(\mathbf{r}_i^2 - x_i^2) - \omega_y x_i y_i - \omega_z x_i z_i] \tag{2}$$

$$L_y = \sum_i m_i[\omega_y(\mathbf{r}_i^2 - y_i^2) - \omega_x x_i y_i - \omega_z y_i z_i] \tag{3}$$

$$L_z = \sum_i m_i[\omega_x(\mathbf{r}_i^2 - z_i^2) - \omega_x x_i y_i - \omega_y y_i z_i] \tag{4}$$

$$\Rightarrow \begin{bmatrix} L_x \\ L_y \\ L_z \end{bmatrix} = \begin{bmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{bmatrix} \begin{bmatrix} \omega_x \\ \omega_y \\ \omega_z \end{bmatrix} \tag{5}$$

Written the equation in the integral form

$$I_{ij} = \int_V \rho(\mathbf{r})\,\mathrm{d}V\,(\mathbf{r}^2\delta_{ij} - r_i r_j) \tag{6}$$

The total kinetic energy is

$$T = \sum_i \frac{1}{2}m_i\mathbf{v}_i^2 = \sum_i \frac{1}{2}m_i(\boldsymbol{\omega} \times \mathbf{r}_i) \cdot \mathbf{v}_i = \frac{1}{2}\boldsymbol{\omega} \cdot \sum_i m_i(\mathbf{r}_i \times \mathbf{v}_i) = \frac{1}{2}\boldsymbol{\omega} \cdot \mathbf{L} = \frac{1}{2}\boldsymbol{\omega}^T I \boldsymbol{\omega} = \frac{1}{2}I_{ij}\omega_i\omega_j \tag{7}$$

If $\boldsymbol{\omega} = \omega\mathbf{n}$, then

$$T = \frac{1}{2}\omega^2\mathbf{n}^T I \mathbf{n} \tag{8}$$

If there is a translational motion

$$\mathbf{v}_i = \mathbf{v}_0 + \boldsymbol{\omega} \times \mathbf{r}_i \tag{9}$$

$$\mathbf{r}_i = \mathbf{r}_0 + \mathbf{r}_i' \tag{10}$$

$$\Rightarrow \mathbf{L} = \sum_i(\mathbf{r}_0 + \mathbf{r}_i') \times (\mathbf{v}_0 + \boldsymbol{\omega} \times \mathbf{r}_i) = M\mathbf{r}_0 \times \mathbf{v}_0 + \sum_i m_i\mathbf{r}_i' \times (\boldsymbol{\omega} \times \mathbf{r}_i') \tag{11}$$

Hence, the kinetic energy becomes (let $\boldsymbol{\omega} = \omega\mathbf{n}$)

$$T = \sum_i \frac{1}{2}m_i(\mathbf{v}_0 + \boldsymbol{\omega} \times \mathbf{r}_i)^2 = \sum_i \frac{1}{2}m_i\mathbf{v}_0^2 + m_i\mathbf{v}_0 \cdot (\boldsymbol{\omega} \times \mathbf{r}_i) + \frac{1}{2}\omega^2 m_i(\mathbf{n} \times \mathbf{r}_i)^2 = \frac{1}{2}M\mathbf{v}_0^2 + \frac{1}{2}I\omega^2 \tag{12}$$

Angular momentum around any point

$$I_a = \sum_i m_i(\mathbf{n} \times \mathbf{r}_i)^2 = \sum_i m_i[\mathbf{n} \times (\mathbf{R} + \mathbf{r}_i')]^2 = \sum_i m_i(\mathbf{n} \times \mathbf{R})^2 + \sum_i m_i(\mathbf{n} \times \mathbf{r}_i')^2 = M(\mathbf{n} \times \mathbf{R})^2 + I_{\mathrm{COM}} \tag{13}$$

5.2 The eigenvalues of the inertia tensor

We can diagonalize the matrix I s.t.

$$I = \begin{bmatrix} I_1 & & \\ & I_2 & \\ & & I_3 \end{bmatrix} \tag{14}$$

The diagonal terms are called the principle moments of inertia, and the axes that diagonalize the matrix are called the principal axes.

Example 5.1 (Uniform cube). For a uniform cube lie in $(0,0,0)$ to (a,a,a), we have

$$I_{xx} = \int_V \rho\,\mathrm{d}V\,(y^2+z^2) = \int_0^a \mathrm{d}x \int_0^a \mathrm{d}y \int_0^a \mathrm{d}z\,(y^2+z^2)\frac{m}{a^3} = \frac{2}{3}ma^2 \tag{15}$$

$$I_{xy} = \int_V \rho\,\mathrm{d}V\, -xy = -\int_0^a \mathrm{d}x \int_0^a \mathrm{d}y \int_0^a \mathrm{d}z xy\frac{m}{a^3} = -\frac{1}{4}ma^2 \tag{16}$$

Hence the inertia tensor is

$$I = \begin{bmatrix} \frac{2}{3} & -\frac{1}{4} & -\frac{1}{4} \\ -\frac{1}{4} & \frac{2}{3} & -\frac{1}{4} \\ -\frac{1}{4} & -\frac{1}{4} & \frac{2}{3} \end{bmatrix} \tag{17}$$

We can first have a guess of eigenvector

$$A_3 = \frac{1}{\sqrt{3}}\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} \tag{18}$$

5.3 Rotational motion of a rigid body

Note that (s means relative to space and b means relative to body)

$$\left(\frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t}\right)_s = \left(\frac{\mathrm{d}\mathbf{L}}{\mathrm{d}t}\right)_b + \boldsymbol{\omega}\times\mathbf{L} = \mathbf{N} \tag{19}$$

Hence we can obtain Euler equations

$$\dot{L}_{bi} + \epsilon_{ijk}\omega_i L_{bk} = N_i \tag{20}$$

$$\Rightarrow \begin{cases} I_1\dot{\omega}_1 - \omega_2\omega_3(I_2-I_3) = N_1 \\ I_2\dot{\omega}_2 - \omega_3\omega_1(I_3-I_1) = N_2 \\ I_1\dot{\omega}_3 - \omega_1\omega_2(I_1-I_2) = N_3 \end{cases} \tag{21}$$

Example 5.2 (Precession with $I_1 = I_2 \neq I_3$). Consider force-free motion of a rigid body with $I_1 = I_2 \neq I_3$, then

$$I_1\dot{\omega}_1 - \omega_2\omega_3(I_2-I_3) = 0 \tag{22}$$

$$I_2\dot{\omega}_2 - \omega_3\omega_1(I_3-I_1) = 0 \tag{23}$$

$$I_3\dot{\omega}_3 = 0 \tag{24}$$

Hence we get

$$\dot{\omega}_1 = \frac{I_1-I_3}{I_1\omega_3}\omega_2 = -\Omega\omega_2 \tag{25}$$

$$\dot{\omega}_2 = \frac{I_3-I_1}{I_1\omega_3}\omega_1 = \Omega\omega_1 \tag{26}$$

$$\omega_3 = \mathrm{const} \tag{27}$$

Hence we can solve the differential equation that

$$\omega_1 = A\cos\Omega t,\ \omega_2 = A\sin\Omega t \tag{28}$$

6 Oscillation

6.1 Formulation

Consider a system with generalize coordinates $q_1, \dots, q_n$ with $3N - k$ DOFs. Let an equilibrium point be

$$\left(\frac{\partial V}{\partial q_i}\right)_{q_i = q_{i0}} = 0 \tag{1}$$

Expand the potential in the 2$^{\text{nd}}$ order

$$V(q_i) = V(q_{0i}) + \left.\frac{\partial V}{\partial q_i}\right|_{q_i = q_{0i}} + \frac{1}{2!}\left.\frac{\partial^2 V}{\partial q_i q_j}\right|_{q_i = q_{0i}} (q_i - q_{0i})(q_j - q_{0j}) + \cdots \tag{2}$$

Define $\eta_i = (q_i - q_{0i})$, then near the equilibrium point we have

$$V(q_i) = \frac{1}{2}\left(\frac{\partial^2 V}{\partial q_i \partial q_j}\right)_0 \eta_i \eta_j = \frac{1}{2} V_{ij} \eta_i \eta_j \tag{3}$$

We can also express the kinetic energy wrt η_i

$$T = \sum_i \frac{1}{2} m_i \dot{\mathbf{r}}_i^2 = \sum_i \frac{1}{2}\left(\frac{\partial \mathbf{r}_i}{\partial t} + \sum_j \frac{\partial \mathbf{r}_i}{\partial \dot{q}_j}\right)^2 = \sum_{ijk} \frac{1}{2} m_i \frac{\partial \mathbf{r}_i}{\partial q_j}\frac{\partial \mathbf{r}_i}{\partial q_k} \dot{q}_j \dot{q}_k = \sum_{jk} \frac{1}{2}\left(\sum_i m_i \frac{\partial \mathbf{r}_i}{\partial q_j}\frac{\partial \mathbf{r}_i}{\partial q_k}\right)\dot{q}_j \dot{q}_k = \sum_{jk} \frac{1}{2} M_{jk} \dot{\eta}_j \dot{\eta}_k \tag{4}$$

Suppose M_{ij} has small variation

$$M_{ij}(q_1, \dots, q_n) = M_{ij}(q_{01}, \dots, q_{0n}) + \left(\frac{\partial M_{ij}}{\partial q_k}\right)\eta_k = M_{ij}(q_{01}, \dots, q_{0n}) = T_{ij} \tag{5}$$

Hence

$$T = \frac{1}{2} T_{ij} \dot{\eta}_i \dot{\eta}_j \tag{6}$$

Therefore we have a Lagrangian

$$L = T - V = \frac{1}{2}(T_i j \eta_i \eta_j - V_{ij} \eta_i \eta_j) \tag{7}$$

The EOM becomes

$$T_{ij} \ddot{\eta}_j + V_{ij} \eta_j = 0 \tag{8}$$

6.2 The eigenvalue equation

Let $\eta_i = C_i e^{-i\omega t}$, we have the EOM

$$V_{ij} C_j - \omega^2 T_{ij} C_j = 0 \tag{9}$$

Write it into the matrix form

$$\begin{bmatrix} V_{11} - \omega^2 T_{11} & \cdots & V_{1n} - \omega^2 T_{1n} \\ \vdots & \ddots & \vdots \\ V_{n1} - \omega^2 T_{n1} & \cdots & V_{nn} - \omega^2 T_{nn} \end{bmatrix} \begin{bmatrix} C_1 \\ \vdots \\ C_n \end{bmatrix} = 0, \ \ \det(\mathbb{V} - \omega^2 \mathbb{T}) = 0 \tag{10}$$

Then we get an eigenvalue equation (note that $\mathbf{C} \in \mathbb{R}^{n \times 1}$)

$$\mathbb{V}\mathbf{C} = \omega^2 \mathbb{T}\mathbf{C} \tag{11}$$

Let ω_α be α^{th} eigenvalue and $\mathbf{C}_\alpha$ be the corresponding eigenvector, then we have

$$\sum_{j=1}^{n}(V_{ij} - \omega_\alpha^2 T_{ij})C_{j\alpha} = 0 \tag{12}$$

$$\sum_{j=1}^{n-1}(V_{ij} - \omega_\alpha^2 T_{ij})C_{j\alpha} = -(V_{in} - \omega_\alpha^2 T_{in})C_{n\alpha} \tag{13}$$

$$\Rightarrow C_{j\alpha} = \frac{\Delta_{jn}}{\Delta_{nn}}C_{n\alpha} \tag{14}$$

where Δ_{ij} is defined as the determinant of a sub-matrix of $\mathbb{A} = \mathbb{V} - \omega_\alpha^2\mathbb{T}$ removing i^{th} row and j^{th} column.
A general solution is a superposition of all the solutions corresponding to a given eigenfrequency

$$\eta_i(t) = \sum_\alpha \eta_{i\alpha}(t) = \sum_\alpha C'_{i\alpha}\underbrace{A_\alpha e^{-i\omega_\alpha t}}_{\xi_\alpha(t)} \tag{15}$$

Hence

$$T = \frac{1}{2}T_{ij}\dot{\eta}_i\dot{\eta}_j = \frac{1}{2}T_{ij}C'_{i\alpha}C'_{j\beta}\dot{\xi}_\alpha\dot{\xi}_\beta \tag{16}$$

$$V = \frac{1}{2}V_{ij}\eta_i\eta_j = \frac{1}{2}V_{ij}C'_{i\alpha}C'_{j\beta}\xi_\alpha\xi_\beta \tag{17}$$

Note that

$$\mathbb{V}\mathbf{C}_\alpha = \omega_\alpha^2\mathbb{T}\mathbf{C}_\alpha \tag{18}$$

$$\mathbb{V}\mathbf{C}_\beta = \omega_\alpha^2\mathbb{T}\mathbf{C}_\beta \tag{19}$$

$$\Rightarrow \mathbf{C}_\beta^T\mathbb{V}\mathbf{C}_\alpha = \omega_\alpha^2\mathbf{C}_\beta^T\mathbb{T}\mathbf{C}_\alpha \tag{20}$$

$$\mathbf{C}_\alpha^T\mathbb{V}\mathbf{C}_\beta = \omega_\beta^2\mathbf{C}_\alpha^T\mathbb{T}\mathbf{C}_\beta \tag{21}$$

$$\Rightarrow (\omega_\alpha^2 - \omega_\beta^2)\mathbf{C}_\beta^T\mathbb{T}\mathbf{C}_\alpha = 0 \tag{22}$$

Hence

$$T_{ij}C_{i\alpha}C_{j\beta} = \delta_{ij} \tag{23}$$

$$T = \frac{1}{2}\dot{\xi}_\alpha\dot{\xi}_\beta\delta_{\alpha\beta} = \frac{1}{2}\dot{\xi}^2 \tag{24}$$

$$V = \frac{1}{2}\omega_\alpha^2\delta_{\alpha\beta}\xi_\alpha\xi_\beta = \frac{1}{2}\omega_\alpha^2\xi_\alpha^2 \tag{25}$$

The EOMs are now

$$\ddot{\xi}_\alpha + \omega_\alpha^2\xi_\alpha = 0 \tag{26}$$

There is no coupling between different ξ_α modes, and ξ_α are called normal coordinates.

Example 6.1. Oscillation of a particle with

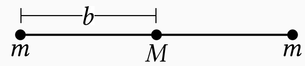
$$V = \frac{1}{2}(k_1x_1^2 + k_2x_2^2 + k_3x_3^2)$$

$$T = \frac{1}{2}m(x_1^2 + x_2^2 + x_3^2)$$

We need to solve the eigenvalue equation $\mathbb{V}\mathbf{C} = \omega^2\mathbb{T}\mathbf{C}$.

$$\begin{bmatrix} k_1 & & \\ & k_2 & \\ & & k_3 \end{bmatrix}\mathbf{C} = \omega^2 m\begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \end{bmatrix}\mathbf{C} \Rightarrow \omega_i = \sqrt{\frac{k_i}{m}},\ i = 1, 2, 3$$

Example 6.2 (Linear triatomic molecule).



We consider vibration along the line of the molecule only. Interactions exist only between atoms neighboring. The equilibrium distance is b. Let $\eta_i = x_i - x_{0i}$ the deviation from the equilibrium point, hence

$$V = \frac{k}{2}(\eta_2 - \eta_1)^2 + \frac{k}{2}(\eta_3 - \eta_2)^2$$
$$T = \frac{m}{2}(\dot{\eta}_1^2 + \dot{\eta}_3^2) + \frac{M}{2}\dot{\eta}_2^2$$

Let COM is at rest, then we can drive that

$$\eta_2 = -\frac{m}{M}(\eta_1 + \eta_3)$$

Then there are only two DOFs left. Define $\xi_1 = \eta_1 + \eta_3$, $\xi_3 = \eta_1 - \eta_3$, then

$$V = \frac{k}{4}\left[\frac{(M+2m)^2}{M^2}\xi_1^2 + \xi_3^2\right]$$
$$T = \frac{m}{4}(\dot{\xi}_1^2 + \dot{\xi}_3^2) + \frac{m^2}{2M}\dot{\xi}_1^2$$

We have two methods to solve the EOM. First, we can consider the Lagrangian. Note that ξ_1 and ξ_3 are independent, which means that we can solve two frequencies independently

$$\omega_1 = \sqrt{\frac{k}{m}\frac{M+2m}{M}},\ \omega_2 = \sqrt{\frac{k}{m}}$$

Or, we can solve it by the eigenvalue equation (wrt eta_i, $i = 1, 2, 3$)

$$\begin{bmatrix} k & -k & 0 \\ -k & 2k & -k \\ 0 & -k & k \end{bmatrix}\mathbf{C} = \omega^2 \begin{bmatrix} m & & \\ & M & \\ & & m \end{bmatrix}\mathbf{C}$$

we can solve three frequencies

$$\omega_1 = 0,\ \omega_2 = \sqrt{\frac{k}{m}\frac{M+2m}{M}},\ \omega_3 = \sqrt{\frac{k}{m}}$$

The zero frequency suggests that $\dot{\xi}_1 = 0$, which corresponds to the translational motion.

In the previous example, we have considered the motion along the molecular axis, i.e., 1D. In more general case, we consider the motion in 3D, then the rigid body DOFs = 6 (3 rotational and 1 translational).

For a general system of n DOFs, there will be $n - 6$ true vibration frequencies/DOFs, and 6 vanishing frequencies corresponding to the rigid body motion or DOFs.

draw figure

Example 6.3 (Vertical vibrations). We assume that there are no COM motions and no COM rotation

$$my_1 + my_2 + my_3 = 0,\ m\dot{y}_1 l - m\dot{y}_3 l = 0 \Rightarrow y_3 = y_1,\ y_2 = -\frac{2m}{M}y_1$$

There is only one DOF y_1 left, the Lagrangian is

$$L = T - V = \frac{m}{M}(M + 2m)\dot{y}_1^2 - \frac{1}{2}k_1 y_1^2$$

Then we can solve the frequency

$$\omega = \sqrt{\frac{k_1 M}{m}(M + 2m)}$$

7 Hamiltonian Equations of Motion

7.1 Legendre transformation

Definition 7.1 (Legendre transformation). Let $\mathrm{d}f = u\,\mathrm{d}x$, the Legendre transformation of f is

$$g = f - ux, \quad \mathrm{d}g = \mathrm{d}f - u\,\mathrm{d}x - x\,\mathrm{d}u = -x\,\mathrm{d}u \tag{1}$$

Example 7.1 (Thermodynamics). Internal energy U

$$\mathrm{d}U = \mathrm{d}Q - P\,\mathrm{d}V = T\,\mathrm{d}S - P\,\mathrm{d}V$$

Enthalpy $H = U + PV$

$$\mathrm{d}H = \mathrm{d}U + P\,\mathrm{d}V + V\,\mathrm{d}P = T\,\mathrm{d}S + V\,\mathrm{d}P$$

Helmholtz free energy $F = U - TS$

$$F = -S\,\mathrm{d}T - P\,\mathrm{d}V$$

Gibbs free energy $G = U - TS + PV$

$$\mathrm{d}G = V\,\mathrm{d}P - S\,\mathrm{d}T$$

The canonical momentum is

$$p_i = \frac{\partial L}{\partial \dot{q}_i} \tag{2}$$

Define Hamiltonian H

$$H(q_i, p_i, t) = p_i\dot{q}_i - L(q_i, \dot{q}_i, t) \tag{3}$$

Hence

$$\begin{aligned}
\mathrm{d}H &= p_i\,\mathrm{d}\dot{q}_i + \dot{q}_i\,\mathrm{d}p_i - \mathrm{d}L && (4)\\
&= p_i\,\mathrm{d}\dot{q}_i + \dot{q}_i\,\mathrm{d}p_i - \frac{\partial L}{\partial q_i}\,\mathrm{d}q_i - \frac{\partial L}{\partial \dot{q}_i}\,\mathrm{d}\dot{q}_i - \frac{\partial L}{\partial t}\,\mathrm{d}t && (5)\\
&= p_i\,\mathrm{d}\dot{q}_i + \dot{q}_i\,\mathrm{d}p_i - \frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}_i}\,\mathrm{d}q_i - p_i\,\mathrm{d}\dot{q}_i - \frac{\partial L}{\partial t}\,\mathrm{d}t && (6)\\
&= \dot{q}_i\,\mathrm{d}p_i - \dot{p}_i\,\mathrm{d}q_i - \frac{\partial L}{\partial t}\,\mathrm{d}t && (7)
\end{aligned}$$

We can get $2n$ 1^{st} order ODEs, which are called Hamilton's equations

$$\begin{aligned}
\dot{q}_i &= \frac{\partial H}{\partial p_i} && (8)\\
\dot{p}_i &= -\frac{\partial H}{\partial q_i} && (9)\\
-\frac{\partial L}{\partial t} &= \frac{\partial H}{\partial t} && (10)
\end{aligned}$$

Standard steps to go from Lagrangian formalism to Hamiltonian formalism

1) Construct $L = L(q_i, \dot{q}_i, t)$ as a function of well-suited generalized coordinates and velocities
2) Derive the generalized/canonical momentum $p_i = \partial L/\partial \dot{q}_i$
3) Do the Legendre transform $H = p_i\dot{q}_i - L$
4) Use p_i to obtain $\dot{q}_i$ as function of $H(q_i, p_i, t)$

Example 7.2 (Particle in a central force field). Choose the generalized coordinates (r, θ, ϕ).

$$L = T - V = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\theta}^2 + r^2\sin^2\theta\dot{\phi}^2) - V(r)$$
$$p_r = m\dot{r},\ p_\theta = mr^2\dot{\theta},\ p_\phi = mr^2\sin^2\theta\dot{\phi}$$

Then the Hamiltonian is

$$H = p_i\dot{q}_i - L = \frac{1}{2m}\left(p_r^2 + \frac{p_\theta^2}{r^2} + \frac{p_\phi^2}{r^2\sin^2\theta}\right) + V$$

Example 7.3 (Particle in a EM field).

$$L = T - U = \frac{1}{2}m\mathbf{v}^2 - q\phi + q\mathbf{A}\cdot\dot{\mathbf{v}} = \frac{1}{2}m\dot{x}_i^2 - q\phi + qA_i\dot{x}_i$$

Then

$$p_i = m\dot{x}_i + qA_i$$
$$H = p_i\dot{x}_i - L = (m\dot{x}_i + qA_i)\dot{x}_i - L = \frac{1}{2}m\dot{x}_i^2 + q\phi = \frac{1}{2m}(p_i - qA_i)^2 + q\phi$$

Example 7.4 (1D harmonic oscillator).

$$L = T - V = \frac{1}{2}m\dot{x}^2 - \frac{1}{2}kx^2,\ p = m\dot{x}$$

Hence

$$H = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

Hamilton's equations are

$$\dot{p} = -kx,\ \dot{x} = \frac{p}{m}$$

Recall the Hamilton's principle of L

$$\delta I = \delta\int_1^2 L\,\mathrm{d}t = 0 \tag{11}$$
$$\Rightarrow \delta I = \delta\int_1^2 \underbrace{(p_i\dot{q}_i - H)}_{f(q_i,\dot{q}_i,p_i,\dot{p}_i,t)}\,\mathrm{d}t = 0 \tag{12}$$

which is called modified Hamilton's principle. Hence, there are two sets of Euler-Lagrange equations

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial f}{\partial\dot{q}_i} - \frac{\partial f}{\partial q_i} = 0 \tag{13}$$
$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial f}{\partial\dot{p}_i} - \frac{\partial f}{\partial p_i} = 0 \tag{14}$$

Then imply that

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \tag{15}$$
$$\dot{q}_i = \frac{\partial H}{\partial p_i} \tag{16}$$

In Lagrangian formalism, the change of variable $q_i \to Q_i(q_j, t)$ does not change the EOM, i.e., they are equivalent. However, in Hamiltonian formalism, the change of coordinate $q_i, p_i \to Q_i, P_i(q_j, p_j, t)$, the transformation cannot be arbitrary, the new variables need to satisfy

$$\dot{P}_i = -\frac{\partial H'}{\partial Q_i} \tag{17}$$

$$\dot{Q}_i = \frac{\partial H'}{\partial P_i} \tag{18}$$

Definition 7.2 (Canonical transformation)**.** The transformation $(q_i, p_i, t) \to (Q_i, P_i, t)$ which preserves Hamilton's equations is called a canonical transformation.

For the old coordinates

$$\delta \int_1^2 p_i \dot{q}_i - H(q, p, t)\, \mathrm{d}t = 0 \tag{19}$$

The new coordinates (should) implies

$$\delta \int_1^2 P_i \dot{Q}_i - H'(Q, P, t)\, \mathrm{d}t = 0 \tag{20}$$

There is a relationship

$$(P_i \dot{Q}_i - H') = \lambda(p_i \dot{q}_i - H) + \frac{\mathrm{d}F}{\mathrm{d}t} \tag{21}$$

where $\delta F_1 = \delta F_2 = 0$, F is called the generating function of canonical transformations. As long as Equation 21 holds, the Hamilton's equations hold. Note that

$$\mathrm{d}F = p_i\, \mathrm{d}q_i - P_i\, \mathrm{d}Q_i + (H' - H)\, \mathrm{d}t,\ F = F(q_i, Q_i, t) \tag{22}$$

$$p_i = \frac{\partial F}{\partial q_i},\ P_i = -\frac{F}{\partial Q_i},\ H = H' - \frac{\partial F}{\partial t} \tag{23}$$

Perform Legendre transformation of P_i and Q_i for F

$$F'(q_i, P_i, t) = F(q_i, Q_i, t) + Q_i P_i \tag{24}$$

$$\Rightarrow \mathrm{d}F' = p_i\, \mathrm{d}q_i + Q_i\, \mathrm{d}P_i + (H' - H)\, \mathrm{d}t \tag{25}$$

Generating function	Derivative relations
$F_1 = F_1(q, Q, t)$	$p_i = \partial F_1 / \partial q_i$, $P_i = -\partial F_1 / \partial Q_i$
$F_2 = F_1(q, Q, t) + Q_i P_i$	$p_i = \partial F_1 / \partial q_i$, $Q_i = \partial F_2 / \partial P_i$
$F_3 = F_1(q, Q, t) - q_i p_i$	$q_i = -\partial F_3 / \partial p_i$, $P_i = -\partial F_3 / \partial Q_i$
$F_4 = F_1(q, Q, t) + Q_i P_i - q_i p_i$	$q_i = -\partial F_4 / \partial p_i$, $Q_i = \partial F_1 / \partial P_i$

Example 7.5 (Identity canonical transformation)**.** Introduce $F_2 = q_i P_i$, then

$$p_i = \frac{\partial F_2}{q_i} = P_i,\ Q_i = \frac{\partial F_2}{P_i} = q_i \tag{26}$$

Example 7.6 (Switch the coordinate and momentum)**.** Let $F_1 = q_i Q_i$, then

$$p_i = \frac{\partial F_1}{\partial q_i} = Q_i,\ P_i = -\frac{\partial F_1}{\partial Q_i} = q_i \tag{27}$$

where we have $(p_, q_i) \to (Q_i = p_i, p_i = -q_i)$.