Contents

1 Lagrangian Mechanics & Formalism

1.1 Principle of Least Action

While Newtonian mechanics uses mainly the geometry of the space to describe and derive motion of objects in this space, constraining the possible paths of the system by Newton's three laws, Lagrangian mechanics chooses a more synthetic approach.
The basic premise of the theory is that behaviour of any mechanical system can be derived from one scalar function of position of components of the system, velocities of the system and time. This function is a called the lagrangian and is denoted as $\mathscr{L}(q_1, q_2, ..., \dot{q}_1, \dot{q}_2, ..., t)$, where q_n is some position coordinate and

$$\dot{q}_n = \frac{dq_n}{dt}$$

is the velocity in this coordinate direction, and t is the time. In order to be able to derive the behaviour of the system from this function, we need to introduce some type of constraints on which paths can the system take. In the case of lagrangian mechanics, the principle of least action is chosen. The action is defined as

$$A = \int_{t_1}^{t_2} \mathscr{L} dt \tag{1}$$

for path from point $q_{11}, q_{21}, ..., t_1$ to $q_{12}, q_{22}, ..., t_2$. The principle of least action (also called Hamilton's principle of least action) then states that out of all paths possible between the two points, the system evolves in a path that minimizes the action A. Later, this principle was generalized to the condition that state chooses simply the action that is extremal - either maximal or minimal.
This is the guiding principle of lagrangian mechanics and we can see that this constraint is much more general than the quite specific Newton's laws. This is also the reason why lagrangian mechanics can be easily extended to include special relativity or quantum mechanics - the principle lagrangian function is simply changed to predict same system paths as given theory and rest of the formalism remains the same.
We will now not go into detail how the lagrangian is derived for different systems, as it will later follow from some of our formalism. To see these derivations, I suggest Landau & Lifshitz Mechanics.
For now, we define the lagrangian in classical mechanics as

$$\mathscr{L} = T - V \tag{2}$$

where T is the total kinetic energy of the system, and V is the total potential energy of the system (both stored and external).
To illustrate the point in a specific example, consider a small object of mass m inside a uniform gravitational field $V = mgx$ in single direction up or down, so that

$$\mathscr{L} = \frac{1}{2}m\dot{x}^2 - mgx$$

The action for it to travel from point (x_1, t_1) to point (x_2, t_2) is

$$A = \int_{t_1}^{t_2} \left(\frac{1}{2}m\dot{x}^2 - mgx\right) dt$$

Assume that the path $x(t)$ leads from (x_1, t_1) to (x_2, t_2) and that it minimizes the action A. Then, assume we add a small variation to the path $\delta x(t)$, such that $\delta x(t_1) = \delta x(t_2) = 0$ and that the function is everywhere very small. If $x(t)$ is truly the minimal path, then A will remain approximately the same for all small variations $\delta x(t)$.
Since the new path is $x'(t) = x(t) + \delta x(t)$, the velocity is $\dot{x}'(t) = \dot{x} + \delta\dot{x}(t)$.
Hence

$$A = \int_{t_1}^{t_2} \left(\frac{1}{2}m(\dot{x} + \delta\dot{x})^2 - mg(x + \delta x)\right)$$

And thus, subtracting the first equation (and disregarding higher order variations $\delta\dot{x}^2$)

$$0 = \int_{t_1}^{t_2} (m\dot{x}\delta\dot{x} - mg\delta x)\, dt$$

The first part of the integral can be integrated by partes as

$$\int_{t_1}^{t_2} m\dot{x}\delta\dot{x}dt = [m\dot{x}\delta x]_{t_1}^{t_2} - \int_{t_1}^{t_2} m\ddot{x}\delta x dt$$

Since we required that $\delta x(t_1) = \delta x(t_2) = 0$, we have

$$[m\dot{x}\delta x]_{t_1}^{t_2} = 0$$

And the integral therefore is

$$\int_{t_1}^{t_2} m\dot{x}\delta\dot{x}dt = -\int_{t_1}^{t_2} m\ddot{x}\delta x dt$$

Substituting into the original integral

$$0 = \int_{t_1}^{t_2} \left(-m\ddot{x} - mg\right)\delta x dt$$

As we can choose any small variation and the equation must still apply, we must have

$$-m\ddot{x} - mg = 0$$

Or

$$\ddot{x} = -g$$

which is known result of steady acceleration in constant gravitational field.

1.2 Euler-Lagrange Equations

Lagrange equations are the result of generalisation of the previous procedure for a general lagrangian $\mathscr{L}(\vec{q}, \dot{\vec{q}}, t)$, where I concantated the different coordinates q_n and velocities $\dot{q}_n$ into a vector $\vec{q}$ and $\dot{\vec{q}}$. Again, consider an optimal path $\vec{q}(t)$ for which

$$A = \int_{t_1}^{t_2} \mathscr{L}(\vec{q}, \dot{\vec{q}}, t)dt$$

A small variation $\delta\vec{q}(t)$ results in a path $\vec{p}(t) = \vec{q}(t) + \delta\vec{q}(t)$ and velocity $\dot{\vec{p}}(t) = \dot{\vec{q}}(t) + \delta\dot{\vec{q}}(t)$.
The lagrangian for this path $\vec{p}$ can be expressed as

$$\mathscr{L}(\vec{p}, \dot{\vec{p}}, t) \approx \mathscr{L}(\vec{q}, \dot{\vec{q}}, t) + \sum_{n=1}^{N} \frac{\partial\mathscr{L}}{\partial q_n}\delta q_n + \sum_{n=1}^{N} \frac{\partial\mathscr{L}}{\partial\dot{q}_n}\delta\dot{q}_n$$

But the action does not change if $\vec{q}(t)$ is the minimal path, so

$$A = \int_{t_1}^{t_2} \mathscr{L}(\vec{q}, \dot{\vec{q}}, t)dt + \int_{t_1}^{t_2} \sum_{n=1}^{N} \frac{\partial\mathscr{L}}{\partial q_n}\delta q_n dt + \int_{t_1}^{t_2} \sum_{n=1}^{N} \frac{\partial\mathscr{L}}{\partial\dot{q}_n}\delta\dot{q}_n dt$$

Subtracting the original equation and assuming that we are dealing with less than infinite amount of dimensions N, we can write

$$0 = \sum_{n=1}^{N} \left(\int_{t_1}^{t_2} \frac{\partial\mathscr{L}}{\partial q_n}\delta q_n dt + \int_{t_1}^{t_2} \frac{\partial\mathscr{L}}{\partial\dot{q}_n}\delta\dot{q}_n dt \right)$$

The second integral by partes is

$$\int_{t_1}^{t_2} \frac{\partial\mathscr{L}}{\partial\dot{q}_n}\delta\dot{q}_n dt = \left[\frac{\partial\mathscr{L}}{\partial\dot{q}_n}\delta q_n\right]_{t_1}^{t_2} - \int_{t_1}^{t_2} \frac{d}{dt}\left(\frac{\partial\mathscr{L}}{\partial\dot{q}_n}\right)\delta q_n dt$$

Again, since we search for path from $(\vec{q}_1, t_1)$ to $(\vec{q}_2, t_2)$, we need that $\delta\vec{q}(t_1) = \delta\vec{q}(t_2) = \vec{0}$, so we have

$$\int_{t_1}^{t_2} \frac{\partial\mathscr{L}}{\partial\dot{q}n}\delta\dot{q}_n dt = -\int_{t_1}^{t_2} \frac{d}{dt}\left(\frac{\partial\mathscr{L}}{\partial\dot{q}_n}\right)\delta q_n dt$$

Hence the original condition becomes

$$0 = \sum_{n=1}^{N} \int_{t_1}^{t_2} \left[\frac{\partial\mathscr{L}}{\partial q_n} - \frac{d}{dt}\left(\frac{\partial\mathscr{L}}{\partial\dot{q}_n}\right)\right]\delta q_n dt$$

Since we can set any variation δq_n to anything small, this equation can only apply for all those δq_n if

$$\forall n : \frac{\partial \mathscr{L}}{\partial q_n} - \frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{q}_n} = 0 \tag{3}$$

These equations are called the Euler-Lagrange equations and are the fundamental building blocks for the lagrangian and hamiltonian mechanics.
Just from using these and considering the symmetry arguments and Galileian transformations, we could derive the form of lagrangian in classical mechanics, but we will not do this here.
It is important to note that the number of dimensions N in the lagrangian does not necesserily indicate the number of spatial dimensions - for example two particle moving in 1 dimension need two coordinates and two velocities to describe them. Generally, the number N is

$$N = \sum_{i=1}^{n} d_i$$

where d_i is the number of spatial dimensions in the ith particle out of n particles move.

1.3 Momentum and force

From the form of lagrangian for classical mechanics for one particle of mass m,

$$\mathscr{L} = \frac{1}{2}m(\vec{\dot{q}})^2 - V(\vec{q})$$

we derive

$$\frac{\partial \mathscr{L}}{\partial q_n} = -\frac{\partial V}{\partial q_n}$$
$$\frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{q}_n} = \frac{d}{dt}m\dot{q}_n$$

Hence

$$-\frac{\partial V}{\partial q_n} = \frac{d}{dt}m\dot{q}_n$$

we can recognize $m\dot{q}_n$ as the components of Newtonian momentum and $-\frac{\partial V}{\partial q_n}$ as components of a Newtonian force. Therefore, we derived Newton's second law

$$\vec{F} = \frac{d\vec{p}}{dt}$$

Hence, we have

$$p_i = \frac{\partial \mathscr{L}}{\partial \dot{q}_i}$$
$$F_i = \frac{\partial \mathscr{L}}{\partial q_i}$$

1.4 Pendulum

The kinetic energy of a small mass on a light rod of fixed length in gravitational field in vertical direction down is

$$T = \frac{1}{2}ml^2\dot{\theta}^2$$

where θ is the angle between the gravitational field direction and the rod. The potential energy is

$$V = mgl(1 - \cos\theta)$$

Hence, the Euler-Lagrange equations are

$$\frac{\partial \mathscr{L}}{\partial \theta} = -\frac{\partial V}{\partial \theta} = mgl\frac{\partial \cos\theta}{\partial \theta} = -mgl\sin\theta$$
$$\frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{\theta}} = \frac{d}{dt}ml^2\dot{\theta} = ml^2\ddot{\theta}$$

$$\frac{\partial \mathscr{L}}{\partial \theta} = \frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{\theta}}$$
$$-mgl\sin\theta = ml^2\ddot{\theta}$$
$$\ddot{\theta} = -\frac{g}{l}\sin\theta$$

We can check by Newtonian mechanics that this is the correct result, and we therefore see the first big advantage of Lagrangian mechanics - we can use a number of different coordinates to describe the location of the objects and the same equations still apply.

1.5 Cycloid

A cycloid is a curve traced by point on a circumference of a rolling circle. It can be parametrically expressed using the total angle rolled by the circle θ as

$$y = R(1+\cos\theta)$$
$$x = R(\theta - \sin\theta)$$

As a coordinate, we can use the distance along the cycloid path, u, with

$$du = \sqrt{dx^2+dy^2} = d\theta\sqrt{\left(\frac{dx}{d\theta}\right)^2+\left(\frac{dy}{d\theta}\right)^2} = Rd\theta\sqrt{(1-\cos\theta)^2+\sin^2\theta} = Rd\theta\sqrt{1-2\cos\theta+1} =$$
$$= \sqrt{2}Rd\theta\sqrt{1-\cos\theta} = \sqrt{2}R\sqrt{2}\sin\left(\frac{\theta}{2}\right)d\theta = 2R\sin\left(\frac{\theta}{2}\right)d\theta$$

We want the u to have 0 at the bottom of the cycloid, where $\theta = \pi$, and to be then increasing in the direction of increasing x. Therefore, we can express u as

$$u = \int_\pi^\theta du = \int_\pi^\theta 2R\sin\left(\frac{\theta}{2}\right)d\theta = 2R\left[-2\cos\left(\frac{\theta}{2}\right)\right]_\pi^\theta = 4R\left(\cos\left(\frac{\pi}{2}\right)-\cos\left(\frac{\theta}{2}\right)\right) = -4R\cos\left(\frac{\theta}{2}\right)$$

Now, consider a particle moving along the cycloidal path in a homogeneous gravitational field. The Lagrangian is

$$\mathscr{L} = T - V = \frac{1}{2}m\dot{u}^2 - mgy = \frac{1}{2}m\dot{u}^2 - mgR(1+\cos\theta) = m\left(\frac{1}{2}\dot{u}^2 - 2gR\cos^2\left(\frac{\theta}{2}\right)\right) = m\left(\frac{1}{2}\dot{u}^2 - \frac{1}{8R}gu^2\right)$$

Hence, the Euler-Lagrange equation is

$$\frac{\partial \mathscr{L}}{\partial u} = \frac{d}{dt}\frac{\partial \mathscr{L}}{\partial \dot{u}}$$
$$-\frac{mgu}{4R} = \frac{d}{dt}m\dot{u}$$
$$\ddot{u} = -\frac{g}{4R}u$$

This is a equation of perfect harmonic motion - while pendulum follows harmonic motion only approximately, particle oscillating on a cycloidal path follows perfect harmonic motion with angular frequency $\sqrt{\frac{g}{4R}}$, independent of amplitude even for big amplitudes.

2 Hamiltonian Mechanics

While Lagrangian mechanics uses positions and velocities of particles, it is often more useful to describe the system in terms of component positions and momenta.
This is done in Hamilton's formulation of mechanics, which starts from the definition of Hamiltonian.

2.1 Hamiltonian

Hamiltonian is defined as

$$H = \left(\sum_i \dot{q}_i \frac{\partial \mathscr{L}}{\partial \dot{q}_i} \right) - \mathscr{L} \tag{4}$$

One important property of Hamiltonian follows from its time dependence

$$\frac{dH}{dt} = \frac{d}{dt} \sum_i \left(\dot{q}_i \frac{\partial \mathscr{L}}{\partial \dot{q}_i} \right) - \frac{d\mathscr{L}}{dt} = \sum_i \left(\frac{d\dot{q}_i}{dt} \frac{\partial \mathscr{L}}{\partial \dot{q}_i} + \dot{q}_i \frac{d}{dt} \frac{\partial \mathscr{L}}{\partial \dot{q}_i} \right) - \frac{\partial \mathscr{L}}{\partial t} - \sum_i \frac{\partial \mathscr{L}}{\partial q_i} \frac{dq_i}{dt} - \sum_i \frac{\partial \mathscr{L}}{\partial \dot{q}_i} \frac{d\dot{q}_i}{dt}$$

Using the Euler-Lagrange equation

$$\frac{dH}{dt} = \sum_i \ddot{q}_i \frac{\partial \mathscr{L}}{\partial \dot{q}_i} + \sum_i \dot{q}_i \frac{\partial \mathscr{L}}{\partial q_i} - \frac{\partial \mathscr{L}}{\partial t} - \sum_i \dot{q}_i \frac{\partial \mathscr{L}}{\partial q_i} - \sum_i \ddot{q}_i \frac{\partial \mathscr{L}}{\partial \dot{q}_i}$$

Hence

$$\frac{dH}{dt} = -\frac{\partial \mathscr{L}}{\partial t} \tag{5}$$

Hence the hamiltonian is only time dependent if the lagrangian is explicitly time dependent, which makes hamiltonian a useful constant for many cases.
Lets further explore the meaning of hamiltonian for a classical system with one particle, where $\mathscr{L} = \frac{1}{2}m\dot{x}^2 - V(x)$. Here

$$H = \dot{x}\frac{\partial \mathscr{L}}{\partial \dot{x}} - \mathscr{L} = \dot{x}m\dot{x} - \frac{1}{2}m\dot{x}^2 + V(x) = \frac{1}{2}m\dot{x}^2 + V(x)$$

Hence, the hamiltonian corresponds to the total energy of the system. Hamiltonian therefore has even a physical interpretation, while lagrangian does not.

2.2 Hamilton's equations

Now, assume that neither hamiltonian nor lagrangian depend explicitly on time. The small change in lagrangian is

$$d\mathscr{L} = \sum_i \frac{\partial \mathscr{L}}{\partial q_i} dq_i + \frac{\partial \mathscr{L}}{\partial \dot{q}_i} d\dot{q}_i$$

Using the definition of canonical momenta $p_i = \frac{\partial \mathscr{L}}{\partial \dot{q}_i}$ and E-L equation

$$d\mathscr{L} = \sum_i \frac{dp_i}{dt} dq_i + p_i d\dot{q}_i = \sum_i \dot{p}_i dq_i + p_i d\dot{q}_i$$

The small change in hamiltonian is

$$dH = \sum_i d(\dot{q}_i p_i) - d\mathscr{L} = \sum_i p_i d\dot{q}_i + \dot{q}_i dp_i - \dot{p}_i dq_i - p_i d\dot{q}_i = \sum_i \dot{q}_i dp_i - \dot{p}_i dq_i$$

But, we could also express the change in hamiltonian explicitly as

$$dH = \sum_i \frac{\partial H}{\partial q_i} dq_i + \frac{\partial H}{\partial p_i} dp_i$$

Hence, we must have for all i

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}, \dot{q}_i = \frac{\partial H}{\partial p_i} \tag{6}$$

These equations are called Hamilton's equations and are an alternative to E-L equations. The main advantage is that these are total of $2N$ first order differential equations, while E-L equations are N second order differential equations.
Also, we can now express the hamiltonian as function of position and momentum, rather than as function of position and velocities, i.e. $H = H(\vec{q}, \vec{p}, t)$

2.3 Hamiltonian Conservation

We already shown that

$$\frac{dH}{dt} = -\frac{\partial \mathscr{L}}{\partial t}$$

However, we are now able to show one more expression for the time change of hamiltonian, using the fact that it can be expressed as function of position and momenta only.

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} + \sum_i \frac{\partial H}{\partial q_i}\dot{q}_i + \frac{\partial H}{\partial p_i}\dot{p}_i$$

Using Hamilton's equations

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} + \sum_i \frac{\partial H}{\partial q_i}\frac{\partial H}{\partial p_i} + \frac{\partial H}{\partial p_i}\left(-\frac{\partial H}{\partial q_i}\right)$$

Therefore

$$\frac{dH}{dt} = \frac{\partial H}{\partial t} \tag{7}$$

The hamiltonian is changing only if it explicitely depends on time.

2.4 Phase Space

Phase space is a useful tool how to visualize possible states accesible to the system. It is a space of canonical coordinates and momenta. So, for particle in 1D motion, the phase space is a space of two dimensions, with one phase coordinate x and other p_x. From the shape of the trajectory of the system in the phase space, some predictions can be made.
For example, for a simple harmonic motion

$$H = \frac{1}{2}m\dot{x}^2 + \frac{1}{2}kx^2 = \frac{p_x^2}{2m} + \frac{1}{2}kx^2$$

Since the hamiltonian does not explicitly depend on time, it is conserved. Therefore, all states on the trajectory in the phase space satisfy

$$\frac{p_x^2}{2mH} + \frac{x^2}{\frac{2H}{k}} = 1$$

This is an equation of an ellipse in the phase space.
The pendulum in phase space behaves similarly for small oscillations. Once the oscillations are big, the shape distorts from the ellipse. For oscillations that go over the top of the pivot, we have two independent oscillating curves above and below the θ axis, one representing continuous movement forward (angle always increasing, p_θ always positive) and the other representing movement backwards.
In case of small oscillations that loose energy over time, we would than expect to see a spiral in the phase space, ending at the origin.

2.5 Conservation Laws

From the form of Hamilton's equation for momentum p_i

$$\dot{p}_i = -\frac{\partial H}{\partial q_i}$$

or Euler-Lagrange equation

$$\dot{p}_i = \frac{\partial \mathscr{L}}{\partial q_i}$$

we can see that if the Lagrangian or Hamiltonian do not explicitly depend on the position q_i, then the momentum p_i is the constant of motion. This is called the Noether's theorem and can be applied generally to any symmetry of the hamiltonian/lagrangian (symmetry meaning that changing some position variable q_i does not change the hamiltonian/lagrangian).
Constants of motion are useful to simplify the equations of motion created by hamiltonian/lagrangian formalism and their connection to symmetry enables us to do only very general considerations before predicting the behaviour of the system.

2.5.1 Multiple Particles

We can describe a system of particles by the same coordinates q_i as follows - first particle has position $(q_{11}, q_{12}, ..., q_{1i}, ...)$, second $(q_{21}, q_{22}, ..., q_{2i}, ...)$ etc. So, the coordinate is generally some q_{ji}, where i goes from 0 to number of spatial dimensions d and j goes from 1 to the number of particles n. Now assume that the interaction potential between the particles only depends on the distance between the particles, i.e. for any two particles k and l

$$V_{kl} = V_{kl}(|\vec{q}_k - \vec{q}_l|)$$

Since the kinetic energy of the particle does not depend on the position of the particles, the force component of a force on particle k from this potential is

$$F_{ki} = \frac{\partial \mathscr{L}}{\partial q_{ki}} = -\frac{\partial V_{kl}}{\partial q_{ki}} = -\frac{\partial V_{kl}(r)}{\partial q_{ki}}$$

where $r = |\vec{q}_k - \vec{q}_l| = \sqrt{(\vec{q}_k - \vec{q}_l)^2}$
Therefore

$$F_{ki} = -\frac{\partial V_{kl}}{\partial r}\frac{\partial r}{\partial q_{ki}} = -\frac{\partial V_{kl}}{\partial r}\frac{q_{ki} - q_{li}}{r}$$

And, the force on the other particle is

$$F_{li} = -\frac{\partial V_{kl}}{\partial q_{li}} = -\frac{\partial V_{kl}}{\partial r}\frac{\partial r}{\partial q_{li}} = \frac{\partial V_{kl}}{\partial r}\frac{q_{ki} - q_{li}}{r} = -F_{ki}$$

Therefore, for any i, we have $F_{ki} = -F_{li}$, or

$$\vec{F}_k = -\vec{F}_l$$

which is otherwise known as Newton's third law. This can be rewritten as

$$\frac{\partial \mathscr{L}}{\partial q_{ki}} + \frac{\partial \mathscr{L}}{\partial q_{li}} = 0$$

This can be extended to general principle for any number of particles as

$$\sum_{j=1}^{n} \frac{\partial \mathscr{L}}{\partial q_{ji}} = 0$$

which is equivalent with (see equations for momentum above)

$$\sum_{j=1}^{n} \frac{\partial H}{\partial q_{ji}} = 0$$

Hence

$$\sum_{j=1}^{n} \frac{d}{dt} p_{ji} = 0$$

$$\frac{d}{dt} \sum_{j=1}^{n} p_{ji} = 0$$

$$\sum_{j=1}^{n} p_{ji} = P_i$$

where P_i is the total momentum of the system in the direction i, which is constant in time. Therefore, the conservation of momentum for these central potentials is transitive.

2.5.2 Symmetries

Now consider a case when the space is somehow symmetrical, so that $\frac{\partial \mathscr{L}}{\partial q_{ji}} = 0$ for all j (but not for all i). Then, the equation

$$\sum_{j=1}^{n} \frac{\partial \mathscr{L}}{\partial q_{ji}} = 0$$

is automatically satisfied and the total momentum in the direction of i is therefore conserved.
Importantly, this is true for both linear momentum and angular momentum, if there are corresponding symmetries in conjugate coordinates.
From this principle, the conservation of angular momentum can be as well derived, considering the spherical polar coordinate system and symmetry in rotation through angle θ or ϕ, respectively.

2.6 Gyroscope

Gyroscopes are objects rotating around one axis and with one pivot at the axis. The position of a gyroscope can be described by three angles - angle θ between the gyroscope axis and the z axis, angle ϕ between the x axis and projection of the gyroscope axis onto the xy plane (these two are analogical with the angles in spherical polar coordinates) and angle β determining the rotation of the gyroscope around its own axis.
Therefore, the angular velocities are $\vec{\omega}_\theta$, which always points perpendicular to the gyroscope, $\vec{\omega}_\phi$, which always points in the $\hat{k}$ direction, and $\vec{\omega}_\beta$, which points along the axis of the gyroscope.
Let l be the distance from the pivot of the gyroscope to its centre of mass, m the mass of the gyroscope, I the moment of inertia of the gyroscope for rotation perpendicular to its axis (around the pivot) and J the moment of inertia for rotation around the gyroscope axis (the β rotation).
While the angular speed $\vec{\omega}_\theta$ is always perpendicular to the gyroscope, the angular speed $\vec{\omega}_\phi$ is not. We can, however, project the angular into perpendicular and parallel directions as

$$\vec{\omega}_\phi = \cos\theta\dot{\phi}\hat{e}_{\omega_\beta} - \sin\theta\dot{\phi}\hat{e}_\theta$$

where $\dot{\phi} = |\vec{\omega}_\phi|$ and $\hat{e}_{\omega_\beta}$ is the unit vector in the direction of the speed $\vec{\omega}_\beta$, which is along the axis of the gyroscope.
The angular velocity due to $\vec{\omega}_\theta$ can be expressed as

$$\vec{\omega}_\theta = \dot{\theta}\hat{e}_\phi$$

And

$$\vec{\omega}_\beta = \dot{\beta}\hat{e}_{\omega_\beta}$$

Therefore, the overall angular velocity is

$$\vec{\omega} = \dot{\theta}\hat{e}_\phi - \sin\theta\dot{\phi}\hat{e}_\theta + (\dot{\beta} + \cos\theta\dot{\phi})\hat{e}_{\omega_\beta}$$

Since all these unit vectors are perpendicular, we can express the total rotational energy as

$$T = \frac{1}{2}\left((\vec{\omega})^2_\phi I_\phi + (\vec{\omega})^2_\theta I_\theta + (\vec{\omega})^2_{\omega_\beta} I_{\omega_\beta}\right) = \frac{1}{2}\left(\dot{\theta}^2 I + \sin^2\theta\dot{\phi}^2 I + (\dot{\beta} + \cos\theta\dot{\phi})^2 J\right)$$

Now, we place the gyroscope into a homogeneous gravitational field. Choosing the plane of zero potential as xy plane, the potential energy is

$$V = mgl\cos\theta$$

Hence, the lagrangian is

$$\mathscr{L} = \frac{1}{2}I[\dot{\theta}^2 + \sin^2\theta\dot{\phi}^2] + \frac{1}{2}J(\dot{\beta} + \cos\theta\dot{\phi})^2 - mgl\cos\theta$$

Since the lagrangian is independent of β and ϕ, the conjugated momenta will be conserved. We now determine all the momenta from the lagrangian

$$p_\theta = \frac{\partial\mathscr{L}}{\partial\dot{\theta}} = I\dot{\theta}$$

$$p_\beta = J(\dot{\beta} + \cos\theta\dot{\phi})$$

$$p_\phi = \frac{\partial\mathscr{L}}{\partial\dot{\phi}} = I\sin^2\theta\dot{\phi} + J(\dot{\beta} + \cos\theta\dot{\phi})\cos\theta = I\sin^2\theta\dot{\phi} + p_\beta\cos\theta$$

Since the lagrangian has no explicit time dependence, the hamiltonian is conserved. As this is a classical system, the hamiltonian is

$$H = T + V = \frac{1}{2}I\dot{\theta}^2 + \frac{1}{2}I\sin^2\theta\dot{\phi}^2 + \frac{1}{2}J(\dot{\beta} + \cos\theta\dot{\phi})^2 + mgl\cos\theta =$$

$$= \frac{1}{2}I\dot{\theta}^2 + \frac{(p_\phi - p_\beta\cos\theta)^2}{2I\sin^2\theta} + \frac{p_\beta^2}{2J} + mgl\cos\theta$$

Therefore, since H, p_ϕ and p_β are all constants

$$\dot{\theta}^2 = \frac{2}{I}\left(H - \left(\frac{(p_\phi - p_\beta\cos\theta)^2}{2I\sin^2\theta} + \frac{p_\beta^2}{2J} + mgl\cos\theta\right)\right) = \frac{2}{I}\left(H - U_{eff}(\theta)\right)$$

where $U_{eff} = \frac{(p_\phi - p_\beta \cos\theta)^2}{2I\sin^2\theta} + \frac{p_\beta^2}{2J} + mgl\cos\theta$ is the effective potentail acting on the gyroscope. Therefore we have a differential equation for the movement of the gyroscope in θ direction

$$\dot{\theta} = \sqrt{\frac{2}{I}(H - U_{eff}(\theta))}$$

The equations of motion for the remaining two coordinates can be derived from the Hamilton's equations

$$\dot{\phi} = \frac{\partial H}{\partial p_\phi} = \frac{p_\phi - p_\beta\cos\theta}{I\sin^2\theta}$$

$$\dot{\beta} = \frac{\partial H}{\partial p_\beta} = \frac{p_\phi - p_\beta\cos\theta}{I\sin^2\theta}(-\cos\theta) + \frac{p_\beta}{J} = \frac{p_\beta}{J} - \dot{\phi}\cos\theta$$

2.7 Motion in Planar Polar Coordinates

Planar Polar coordinates are defined as

$$r = \sqrt{x^2+y^2}, \phi = \tan^{-1}\left(\frac{y}{x}\right)$$

Or inversly

$$x = r\cos\phi, y = r\sin\phi$$

The unit vectors $\hat{e}_r$ and $\hat{e}_\phi$ are

$$\hat{e}_r = \frac{\frac{d\vec{r}}{dr}}{\left|\frac{d\vec{r}}{dr}\right|} = \cos\phi\hat{i} + \sin\phi\hat{j}$$

$$\hat{e}_\phi = \frac{\frac{d\vec{r}}{d\phi}}{\left|\frac{d\vec{r}}{d\phi}\right|} = -\sin\phi\hat{i} + \cos\phi\hat{j}$$

We can easily see that these two are orthogonal. We can also see that the position vector is

$$\vec{r} = r\hat{e}_r$$

The velocity vector is

$$\vec{v} = \frac{d\vec{r}}{dt} = \dot{r}\hat{e}_r + r\frac{d\hat{e}_r}{dt} = \dot{r}\hat{e}_r + r\dot{\phi}\hat{e}_\phi$$

Hence the kinetic energy of a particle is

$$T = \frac{1}{2}m(\vec{v})^2 = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\phi}^2)$$

Hence the classical hamiltonian is

$$H = T + V = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\phi}^2) + V(r,\phi)$$

We therefore have four hamilton's equations - two for r and two for ϕ coordinates and momenta. For r

$$\dot{p}_r = -\frac{\partial H}{\partial r}$$

$$\dot{r} = \frac{\partial H}{\partial p_r}$$

And for ϕ

$$\dot{p}_\phi = -\frac{\partial H}{\partial \phi}$$

$$\dot{\phi} = \frac{\partial H}{\partial p_\phi}$$

An important observation is that if $V = V(r)$, i.e. V is a central potential, then $\dot{p}_\phi = 0$ and p_ϕ is conserved.

To find p_r and p_ϕ, we use explicit derivation from the lagrangian

$$\mathscr{L} = \frac{1}{2}m(\dot{r}^2 + r^2\dot{\phi}^2) - V(r,\phi)$$

$$p_r = \frac{\partial \mathscr{L}}{\partial \dot{r}} = m\dot{r}$$

$$p_\phi = \frac{\partial \mathscr{L}}{\partial \dot{\phi}} = mr^2\dot{\phi}$$

Hence, the hamiltonian can be rewritten as

$$H = \frac{p_r^2}{2m} + \frac{p_\phi^2}{2mr^2} + V(r,\phi)$$

Hence

$$\dot{p}_\phi = -\frac{\partial V}{\partial \phi}$$

$$\dot{p}_r = \frac{p_\phi^2}{mr^3} - \frac{\partial V}{\partial r}$$

2.7.1 Central Potential

In central potentials, p_ϕ is a constant, hence we can the hamiltonian in this potential can be written as

$$H = \frac{p_r^2}{2m} + \frac{p_\theta^2}{2mr^2} + V(r) = \frac{p_r^2}{2m} + V_c(r) + V(r) = \frac{p_r^2}{2m} + U_{eff}(r)$$

where $U_{eff} = V_c(r) + V(r)$ is the effective potential and $V_c(r)$ is the centrifugal potential. To understand the centrifugal potential, we can have a look at the change of momentum p_r

$$\dot{p}_r = \frac{p_\phi^2}{mr^3} - \frac{\partial V}{\partial r} = -\frac{\partial V_c}{\partial r} - \frac{\partial V}{\partial r} = -\frac{\partial U_{eff}}{\partial r}$$

Therefore, the centrifugal potential demonstrates itself as an additional force that is added to the force due to the potential V. As the centrifugal potential is decreasing with increasing r, its derivative is negative and therefore the force (which is in opposite direction than the derivative) points always in the direction of the radial vector - in direction of increasing r.
Because the hamiltonian does not explicitly depend on time, it is conserved, and thus

$$H = const. = \frac{p_r^2}{2m} + U_{eff}(r)$$

$$p_r = \sqrt{2m(H - U_{eff}(r))}$$

2.7.2 Coulomb Potential

Among many possible forms of potential, potential of type $V(r) = -\frac{\alpha}{r}$ has special importance, as it represents both gravitational potential and potential of electric field, both from a point source.
The effective potential is then

$$U_{eff} = \frac{p_\phi^2}{2mr^2} - \frac{\alpha}{r} = \frac{p_\phi^2}{2m}\left(\frac{1}{r^2} - 2\frac{\alpha m}{p_\phi^2}\frac{1}{r}\right) = \frac{p_\phi^2}{2m}\left[\left(\frac{1}{r} - \frac{\alpha m}{p_\phi^2}\right)^2 - \frac{\alpha^2 m^2}{p_\phi^4}\right]$$

$$U_{eff} = \frac{p_\phi^2}{2m}\left(\frac{1}{r} - \frac{m\alpha}{p_\phi^2}\right)^2 - \frac{\alpha^2 m}{2p_\phi^2}$$

at infinity, this goes to zero, at zero, this goes to infinity.
Also, there is a minimum of the effective potential at

$$\frac{1}{r_{min}} = \frac{m\alpha}{p_\phi^2}$$

$$r_{min} = \frac{p_\phi^2}{m\alpha}$$

where

$$U_{min} = -\frac{\alpha^2 m}{2p_\phi^2}$$

We can now qualitatively see that if the total energy is higher than the minimum energy, the particle will somehow oscillate, unless the energy of the particle is so big that it can escape the potential through increasing r.
Dependent on the particle energy, if the particle is bound ($H < 0$), it follows eliptical orbits, if the particle has $H = 0$, it follows a parabolic orbit, and if $H > 0$, particle follows hyperbolic orbit. As a special case of eliptical orbit, for $H = U_{min}$, the particle follows circular orbit (in the diagram of U_{eff}, it sits in the only potential well on the bottom).

3 Matrices

3.1 Inertia Matrix

Consider a case when we describe a system of two particles with coordinates q_1, which describes the position of particle one with respect to immobile origin, and q_2, which is relative position of particle two with respect to particle one. This means that the position of particle two with respect to origin is

$$q_2' = q_2 + q_1$$

Hence the speed of the particle two is

$$\dot{q}_2' = \dot{q}_2 + \dot{q}_1$$

Hence the kinetic energy of both particles is

$$T = \frac{1}{2}m_1\dot{q}_1^2 + \frac{1}{2}m_2(\dot{q}_2')^2 = \frac{1}{2}m_1\dot{q}_1^2 + \frac{1}{2}m_2(\dot{q}_1 + \dot{q}_2)^2$$

Hence the momentum in the direction q_1 (assuming no dependence of V on speed) is

$$p_1 = \frac{\partial \mathscr{L}}{\partial \dot{q}_1} = \frac{\partial T}{\partial q_1} = m_1\dot{q}_1 + m_2(\dot{q}_1 + \dot{q}_2) = (m_1 + m_2)\dot{q}_1 + m_2\dot{q}_2$$

We can now see that the coefficient in front of $\dot{q}_1$ is not dependent only on the properties of particle one - there is some coupling with the other particle.
To generalize this notion of coupling, we could define the general momentum in direction i for j particles as

$$p_i = \sum_j M_{ij}\dot{q}_j$$

where M_{ij} is some coefficient with dimensions of mass. We can clearly recognize the matrix structure in this notation, and hence we could write

$$\vec{p} = \mathbf{M}\vec{\dot{q}} \tag{8}$$

where matrix multiplication is implied and $\vec{p}$ and $\vec{\dot{q}}$ are column vectors.
How do we find the the elements of $\mathbf{M}$? From the definition of canonical momentum (for V independent of velocities)

$$p_i = \frac{\partial T}{\partial \dot{q}_i} = \sum_j M_{ij}\dot{q}_j$$

We can now differentiate with respect ot $\dot{q}_k$

$$\frac{\partial^2 T}{\partial \dot{q}_i \partial \dot{q}_k} = \sum_j M_{ij}\frac{\partial \dot{q}_j}{\partial \dot{q}_k} = \sum_j M_{ij}\delta_{jk} = M_{ik}$$

where δ_{ik} is the Kronecker delta.
Therefore, we have found the relation for matrix elements of M_{ij} as

$$M_{ij} = \frac{\partial^2 T}{\partial q_i \partial q_j} \tag{9}$$

Hence, we can already see that M_{ij} is a symmetrical matrix, as

$$M_{ij} = \frac{\partial^2 T}{\partial q_i \partial q_j} = \frac{\partial^2 T}{\partial q_j \partial q_i} = M_{ji}$$

We derived the inertia matrix from the expression for momentum, but we can in fact define it only for kinetic energy as

$$T = \frac{1}{2}\vec{q} \cdot \vec{p} = \frac{1}{2}\sum_i \sum_j q_i M_{ij} q_j$$

We can easily check that this definition satisfies the momentum equation and thus is a wider definition of **M**, which we call the inertia matrix.

3.2 Force Matrix

Consider a potential only dependent on the canonical coordinates $V = V(\vec{q})$. Also, consider that the potential has a minimum at $\vec{q_0}$. This means that

$$\forall i : \left.\frac{\partial V}{\partial q_i}\right|_{\vec{q}=\vec{q_0}} = 0$$

Now, consider a small perturbation from the equilibrium position $\vec{r}$. Using Taylor series, we can expend the potential as

$$V(\vec{q_0} + \vec{r}) \approx V(\vec{q_0}) + \sum_i \left.\frac{\partial V}{\partial q_i}\right|_{\vec{q}=\vec{q_0}} r_i + \frac{1}{2}\sum_i \sum_j \left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_{\vec{q}=\vec{q_0}} r_i r_j$$

Since we are at equilibrium, the previous equation becomes

$$V(\vec{q_0} + \vec{r}) \approx V(\vec{q_0}) + \frac{1}{2}\sum_i \sum_j \left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_{\vec{q}=\vec{q_0}} r_i r_j$$

If the kinetic energy T does not depend explicitly on the position $\vec{r}$, we can write the canonical force corresponding to perturbation r_k as

$$F_k = \frac{\partial \mathscr{L}}{\partial r_k} = -\frac{\partial V}{\partial r_k} = -\frac{1}{2}\sum_i \sum_j \left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_{\vec{q}=\vec{q_0}} \left(r_i \frac{\partial r_j}{\partial r_k} + r_j \frac{\partial r_i}{\partial r_k}\right) =$$

$$= -\frac{1}{2}\sum_i \sum_j \left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_{\vec{q}=\vec{q_0}} r_i \delta_{jk} - \frac{1}{2}\sum_i \sum_j \left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_{\vec{q}=\vec{q_0}} r_j \delta_{ik} =$$

$$= -\frac{1}{2}\left[\sum_i \left.\frac{\partial^2 V}{\partial q_i \partial q_k}\right|_{\vec{q}=\vec{q_0}} r_i + \sum_j \left.\frac{\partial^2 V}{\partial q_k \partial q_j}\right|_{\vec{q}=\vec{q_0}} r_j\right] = -\frac{1}{2}\left[2\sum_j \left.\frac{\partial^2 V}{\partial q_j \partial q_k}\right|_{\vec{q}=\vec{q_0}} r_j\right]$$

We could then write

$$F_i = -\sum_j \left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_{\vec{q}=\vec{q_0}} r_j$$

We can again recognize the matrix form of this notation, and write (now choosing r coordinates as the primary coordinates, and origin at the position of $\vec{q_0}$, so that $r_i \to q_i$ and $\vec{q_0} \to \vec{0}$)

$$\vec{F} = -\mathbf{K}\vec{q} \tag{10}$$

where the elements of **K** are

$$K_{ij} = \left.\frac{\partial^2 V}{\partial q_i \partial q_j}\right|_{\vec{q}=\vec{0}} \tag{11}$$

We again see that the matrix is symmetrical.

3.3 Secular Equation

We showed that the canonical momenta can be expressed as

$$\vec{p} = \mathbf{M}\dot{\vec{q}}$$

Similarly, the force elements are for small deviations from a minimum

$$\vec{F} = -\mathbf{K}\vec{q}$$

By Euler-Lagrange equations, we have

$$\vec{F} = \frac{d}{dt}\vec{p}$$

If we assume constant $\mathbf{M}$

$$\vec{F} = \mathbf{M}\ddot{\vec{q}}$$
$$\mathbf{K}\vec{q} = -\mathbf{M}\ddot{\vec{q}} \tag{12}$$

This is a set of equations of motion, that are coupled together. We can try a solution in form of

$$\vec{q} = A\vec{X}e^{i\omega t}$$

where $\vec{X}$ is some vector giving relative directions of motion of separate particles (constant), A is some amplitude and ω is some angular frequency. Then

$$\ddot{\vec{q}} = -A\omega^2\vec{X}e^{i\omega t} = -\omega^2\vec{q}$$

The equation of motion is then

$$\mathbf{K}\vec{q} = \mathbf{M}\omega^2\vec{q}$$

Hence, we have

$$(\mathbf{K} - \omega^2\mathbf{M})\vec{q} = 0$$

and

$$(\mathbf{K} - \omega^2\mathbf{M})\vec{X} = 0 \tag{13}$$

This equation is called the secular equation and has close resemblance to the eigenvalue equation for matrices. It can be solved exactly analogously. First step is to discover that in order for some linear combination of columns of $\mathbf{K}-\omega^2\mathbf{M}$ to sum to zero, at least one of the columns must be a linear superposition of the others. But, since multiplication by column vector from right is nothing else than creating a linear superposition of the matrix columns, this is exactly what the secular equation states.
Since the columns of $\mathbf{K} - \omega^2\mathbf{M}$ are not linearly independent the determinant of the matrix is zero, i.e.

$$|\mathbf{K} - \omega^2\mathbf{M}| = 0 \tag{14}$$

These two equations can be used to find all ω and $\vec{X}$ and thus all solutions of form

$$\vec{q}_\omega = A_\omega\vec{X}_\omega e^{i\omega t}$$

These solutions are called the normal modes of oscillations of the system. Sometimes, it is also just the vector $\vec{X}_\omega$ which is reffered to as the normal mode.
Since there is a specified amplitude A_ω that is unknown, we can choose $\vec{X}_\omega$ either normalized or such that is useful for us, without the loss of generality (because secular equation leads to an infinite amount of scalar multiples of some vector $\vec{X}_\omega$).
Other important property of the equation of motion is its linearity. Assume that $\vec{q}_\omega$ and $\vec{q}_\nu$ are both normal modes, i.e.

$$(\mathbf{K} - \omega^2\mathbf{M})\vec{q}_\omega = 0, (\mathbf{K} - \nu^2\mathbf{M})\vec{q}_\nu = 0$$

Now, consider a linear superposition $\vec{q} = a\vec{q}_\omega + b\vec{q}_\nu$. Substituting this solution into the equation of motion

$$\mathbf{K}\vec{q} = -\mathbf{M}\ddot{\vec{q}}$$

For any normal mode, $\ddot{\vec{q}} = -\omega^2\vec{q}$. Hence

$$\mathbf{K}(a\vec{q}_\omega + b\vec{q}_\nu) = \mathbf{M}(a\omega^2\vec{q}_\omega + b\nu^2\vec{q}_\nu)$$

This leads to

$$a(\mathbf{K} - \omega^2\mathbf{M})\vec{q}_\omega + b(\mathbf{K} - \nu^2\mathbf{M})\vec{q}_\nu = 0$$

but comparing this to the normal modes equations confirms that this equation is true, hence that the superposition $\vec{q}$ is also a solution of the equation of motion. Hence, the general motion of the system can be expressed as linear superposition of the normal modes of the oscillations.
As a consequence of this, we require that normal modes are orthogonal.

3.4 Normal Modes and Symmetry

If there is a symmetry present in the system, we would expect the normal mode vectors $\vec{X}_\omega$ to obey this symmetry. If we can express the symmetry operation by matrix $\mathbf{S}$, then we would expect the symmetry operation to change the $\vec{X}_\omega$ only by some scalar constant λ, so that

$$\mathbf{S}\vec{X}_\omega = \lambda\vec{X}_\omega$$

or

$$(\mathbf{S} - \lambda\mathbf{I})\vec{X}_\omega = 0$$

where $\mathbf{I}$ is the identity matrix. This is the classical eigenvalue equation, and shows that we would expect the vectors of the normal modes to be eigenvectors of the symmetry matrix $\mathbf{S}$. In general, we could replace the matrix $\mathbf{S}$ by some general operator $\hat{S}$ and require

$$\hat{S}\vec{X}_\omega = \lambda\hat{I}\vec{X}_\omega$$

where $\hat{I}$ is the identity operator.
This consideration can help us find the normal modes vectors without solving the secular equation, as solving for eigenvalues of $\mathbf{S}$ is usually much easier than solving the secular equation.
However, the results should be checked, as sometimes the symmetry does not give all normal modes or does not predict exact value of each component of a normal mode vector.
Finally, for a motion with N generalized coordinates (sum of number of dimensions of motion for each particle), we should expect N normal modes for the system (as the motion of the system cannot loose the information about the dimensions).

3.5 Normal Modes Examples

3.5.1 Two Masses between Walls

Imagine following setup : two bodies of identical mass m are attached to three springs as follows. Spring one leads from an immobile wall to first mass and has stiffness k, second leads from the first mass to the second mass and has stiffness k_{12} and the last one leads to the immobile wall and has stiffness k again.
The position of masses can be given in their displacement from walls. Let x_1 be the position of mass one and x_2 position of mass two. The kinetic energy of the system can be described as

$$T = \frac{1}{2}m\dot{x}_1^2 + \frac{1}{2}m\dot{x}_2^2$$

The potential energy can be described as

$$V = \frac{1}{2}kx_1^2 + \frac{1}{2}kx_2^2 + \frac{1}{2}k_{12}(x_1 - x_2)^2$$

Hence the inertia matrix is

$$\mathbf{M} = \begin{pmatrix} m & 0 \\ 0 & m \end{pmatrix}$$

as the masses are not coupled. The force matrix is

$$\mathbf{K} = \begin{pmatrix} k + k_{12} & -k_{12} \\ -k_{12} & k + k_{12} \end{pmatrix}$$

The secular equation is

$$(\mathbf{K} - \omega^2\mathbf{M})\vec{X}_\omega = 0$$

The system is clearly invariant under the exchange of particle one and two.
This means that the permutation matrix $\mathbf{P}_{12}$

$$\mathbf{P}_{12} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

is the symmetry matrix for the system. Hence, the normal modes should be the eigenvectors of this permutation matrix. We can recognize $\mathbf{P}_{12}$ as Pauli matrix σ_1, with known eigenvalues and eigenvectors. For exercise, these are again derived here. The eigenvalues of $\mathbf{P}_{12}$ must satisfy

$$\begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = 0$$

$$\lambda = \pm 1$$

The eigenvectors must satisfy

$$\begin{pmatrix} \mp 1 & 1 \\ 1 & \mp 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

which leads to two eigenvectors $\begin{pmatrix} 1 \\ \pm 1 \end{pmatrix}$

To verify these eigenvectors, we use secular equation

$$(\mathbf{K} - \omega^2 \mathbf{M})\vec{X}_\omega = 0$$

$$\begin{pmatrix} k_1 + k_{12} - \omega^2 m & -k_{12} \\ -k_{12} & k_1 + k_{12} - \omega^2 m \end{pmatrix} \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} = \begin{pmatrix} k_1 + k_{12} - \omega^2 m \mp k_{12} \\ -k_{12} \pm k_1 \pm k_{12} \mp \omega^2 m \end{pmatrix} =$$

$$= \begin{pmatrix} 1 \\ \pm 1 \end{pmatrix} (k_1 + k_{12} - \omega^2 m \mp k_{12})$$

This means that the secular equation applies if

$$\omega^2 m = k_1 + k_{12} \mp k_{12}$$

Hence

$$\omega = \sqrt{\frac{k_1 + k_{12} \mp k_{12}}{m}}$$

Therefore, we have one low frequency symmetrical mode and one high frequency anti-symmetrical mode.

3.5.2 Carbon Dioxide Molecule

We can model carbon dioxide molecule as three colinear masses with masses $m_1 = m_3 = m_O$ and $m_2 = m_C$, which are connected by springs of equal stiffness k, with m_1 connected to m_2 and m_3 connected to m_2. Let x_C be the coordinate of the mass m_2, x_3 coordinate of mass m_3 relative to m_2 and x_1 the coordinate of mass m_1 with respect to mass m_2, taken in the same direction. The kinetic energy is then

$$T = \frac{1}{2} m_O (\dot{x}_1 + \dot{x}_C)^2 + \frac{1}{2} m_C \dot{x}_C^2 + \frac{1}{2} m_O (\dot{x}_3 + \dot{x}_C)^2$$

The inertia matrix is

$$\mathbf{M} = \begin{pmatrix} m_O & m_O & 0 \\ m_O & 2m_O + m_C & m_O \\ 0 & m_O & m_O \end{pmatrix}$$

The potential energy is

$$V = \frac{1}{2} k x_1^2 + \frac{1}{2} k x_3^2$$

Hence the stiffness matrix is

$$\mathbf{K} = \begin{pmatrix} k & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & k \end{pmatrix}$$

There is a symmetry to the exchange of the oxygen atoms, with permutation matrix $\mathbf{P}_{13}$ as the symmetry matrix

$$\mathbf{P}_{13} = \begin{pmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{pmatrix}$$

To find the eigenvalues of $\mathbf{P}_{13}$

$$\begin{vmatrix} -\lambda & 0 & 1 \\ 0 & 1-\lambda & 0 \\ 1 & 0 & -\lambda \end{vmatrix} = (1-\lambda) \begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = -(\lambda - 1)(\lambda^2 - 1) = 0$$

$$(\lambda - 1)^2 (\lambda + 1) = 0$$

which means that we have some degenerate eigenvectors with eigenvalue 1 and non-degenerate eigenvector with eigenvalue -1. For the non-degenerate eigenvector

$$\begin{pmatrix} 1 & 0 & 1 \\ 0 & 2 & 0 \\ 1 & 0 & 1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Which corresponds to eigenvector $\vec{X}_1 = \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix}$. This is the common oscillation of the two oxygen atoms in opposite direction - the anti-symmetric mode (hence eigenvalue -1).
The degenerate eigenvectors need to satisfy

$$\begin{pmatrix} -1 & 0 & 1 \\ 0 & 0 & 0 \\ 1 & 0 & -1 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

which leads to set of eigenvectors $\begin{pmatrix} 1 \\ b \\ 1 \end{pmatrix}$, where b can be any constant. This set has orthogonal basis consisting of two vectors

$$\vec{X}_2 = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \vec{X}_3 = \begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}$$

The first vector corresponds to the translational mode, and the second to the oscillations of C and O atoms in opposite direction.
To check these, start with the non-degenerate eigenvector

$$(\mathbf{K} - \omega_1^2 \mathbf{M})\vec{X}_1 = \vec{0}$$

$$\begin{pmatrix} k - \omega_1^2 m_O & -\omega_1^2 m_O & 0 \\ -\omega_1^2 m_O & -\omega_1^2(2m_0 + m_C) & -\omega_1^2 m_O \\ 0 & -\omega_1^2 m_O & k - \omega_1^2 m_O \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

This clearly only works if $\omega_1 = \sqrt{\frac{k}{m_O}}$.
For translational motion is

$$\begin{pmatrix} k - \omega_2^2 m_O & -\omega_2^2 m_O & 0 \\ -\omega_2^2 m_O & -\omega_2^2(2m_0 + m_C) & -\omega_2^2 m_O \\ 0 & -\omega_2^2 m_O & k - \omega_2^2 m_O \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

this clearly requires $\omega_2 = 0$, which is expected of the translational mode.
We could try the same for the other vector, but we would find a problem - the requirement would be for frequency to be the same as ω_1. Therefore, the last normal mode is not accesible from the symmetry arguments. Therefore, we need to solve for determinant of $\mathbf{K} - \omega^2 \mathbf{M}$ explicitly

$$|\mathbf{K} - \omega^2 \mathbf{M}| = 0$$

$$(k - \omega^2 m_O) \begin{vmatrix} -\omega^2(2m_O + m_C) & -\omega^2 m_O \\ -\omega^2 m_O & k - \omega^2 m_O \end{vmatrix} + \omega^2 m_O \begin{vmatrix} -\omega^2 m_O & -\omega^2 m_O \\ 0 & k - \omega^2 m_O \end{vmatrix} = 0$$

$$-(k - \omega^2 m_O)(\omega^2(2m_O + m_C)(k - \omega^2 m_O) + \omega^4 m_O^2) - (k - \omega^2 m_O)\omega^4 m_O^2 = 0$$

We are not interested in solution $\omega = 0$ or $k - \omega^2 m_O = 0$, so we are left with

$$(2m_O + m_C)(k - \omega^2 m_O) + 2\omega^2 m_O^2 = 0$$

$$(2m_O + m_C)k - 2m_O^2\omega^2 - m_C m_O \omega^2 + 2\omega^2 m_O^2 = 0$$

$$(2m_O + m_C)k = m_C m_O \omega^2$$

Hence

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

To find the normal mode vector

$$\begin{pmatrix} k-\frac{(2m_O+m_C)k}{m_C} & -\frac{(2m_O+m_C)k}{m_C} & 0 \\ -\frac{(2m_O+m_C)k}{m_C} & -\frac{(2m_O+m_C)^2k}{m_Om_C} & -\frac{(2m_O+m_C)k}{m_C} \\ 0 & -\frac{(2m_O+m_C)k}{m_C} & k-\frac{(2m_O+m_C)k}{m_C} \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

From the first and third row, we see that $a = c$. From the second row then

$$2\frac{(2m_O+m_C)k}{m_C}a = -\frac{(2m_O+m_C)^2k}{m_Om_C}c$$

Hence

$$c = -\frac{2m_O}{(2m_O+m_C)}a$$

And the eigenvector is

$$\vec{X}_3 = \begin{pmatrix} 1 \\ -\frac{2m_O}{(2m_O+m_C)} \\ 1 \end{pmatrix}$$

we therefore see that this normal vector lies in the space of eigenvectors of $\mathbf{P}_{13}$, specifically in the subspace created by the degenerate eigenvectors.