Theoretical Physics 2 - Summary

Classical Mechanics

Generalised Description of Mechanical Systems

Dynamical Variables

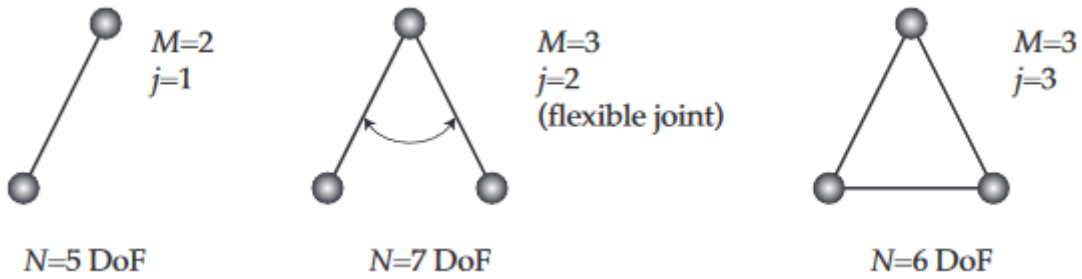
These are any set of variables that completely describe the configuration of a mechanical system. In 3D space possible sets include (x, y, z), (r, ϕ, z) and (r, θ, ϕ).

The **equation of motion** of a system specifies the dynamical variables as functions of time.

Degrees of Freedom (DoF)

The motion of a point mass $\mathbf{r}(t)$ is described by three *independent* dynamical variables, i.e. the point mass has $N = 3$ DoF.

A system of M point masses has $N = 3M$ DoF, but the existence of j *independent* constraints reduced this number to $N = 3M - j$ DoF.



Types of constraints

If constraints on a system of M point masses can be expressed in the form

$$f(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_M, t) = 0$$

Then the constraints are called **holonomic**:

- **Rheonomic** constraints have an explicit time dependence.
- **Scleronomic** constraints do no, i,e, $f(\mathbf{r}_1, \mathbf{r}_2, \ldots, \mathbf{r}_M) = 0$

Nonholonomic constraints involve either differential equations or inequalities (rather than algebraic equations).

Generalised Coordinates

The existence of j constraints means that the coordinates are no longer independent.

We require only as many generalised coordinates q_k as there are DoF.

If the constraints are holonomic, then the position of the ith part of the system can be expressed as:

$$\mathbf{r}_i = \mathbf{r}_i(q_1, \dots, q_k, \dots, q_N, t)$$

The generalised velocities are:

$$\dot{q}_k = \frac{\mathrm{d}q_k}{\mathrm{d}t}$$

q_k and $\dot{q}_k$ are independent variables, so

$$\frac{\partial q_k}{\partial \dot{q}_k} = \frac{\partial \dot{q}_k}{\partial q_k} = 0$$

By the chain rule, we can derive the following:

$$\mathbf{v}_i = \dot{\mathbf{r}}_i = \sum_k \frac{\partial \mathbf{r}_i}{\partial q_k}\dot{q}_k + \frac{\partial \mathbf{r}_i}{\partial t} \implies \frac{\partial \dot{\mathbf{r}}_i}{\partial \dot{q}_k} = \frac{\partial \mathbf{r}_i}{\partial q_k}$$

This last step is known as "cancelling the dots".

The Lagrangian

Lagrange's Formulation of Mechanics

Make three assumptions:

1. Holonomic constants
2. Constraining forces do no virtual work
3. Applied forces are conservative such that a scalar potential energy function exists

D'Alembert's Principle

Newton's 2nd Law for particle i is:

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

Implying that:

$$\sum_i (\mathbf{F}_i - \dot{\mathbf{p}}_i) \cdot \delta\mathbf{r}_i = 0$$

Where $\delta\mathbf{r}_i$ represents an arbitrary virtual displacement (a hypothetical change of coordinates at one instant in time that is compatible with the constraints).

The force includes both the constraint and applied forces such that:

$$\mathbf{F}_i = \mathbf{F}_i^{(c)} + \mathbf{F}_i^{(a)}$$

But since the constraining forces do no virtual work, D'Alembert's Principle is given as:

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

Generalised Equations of Motion

The Lagrangian is defined as:

$$\mathcal{L} = T - V$$

The Euler-Lagrange equations are then:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_k}\right) - \frac{\partial \mathcal{L}}{\partial q_k} = 0$$

Where $\mathcal{L} = \mathcal{L}(q_k, \dot{q}_k, t)$.

Ignorable Coordinates

If the time derivative of a coordinate appears in the Lagrangian, but the coordinate itself does not, then this is an ignorable coordinates. Since

$$\frac{\partial \mathcal{L}}{\partial q_k} = 0$$

the Euler-Lagrange equation implies that:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial \mathcal{L}}{\partial \dot{q}_k}\right) = 0$$

Thus, the **canonically conjugate momentum** to the coordinates, defined as

$$p_k = \frac{\partial \mathcal{L}}{\partial \dot{q}_k}$$

is a constant of the motion.

Variational Calculus

Calculus of Variations

To find the path $y(x)$ which yields the extreme value of the functional:

$$I[y] = \int_{x_1}^{x_2} f(y, y', x)\mathrm{d}x$$

where $y' = \mathrm{d}y/\mathrm{d}x$, the Euler-Lagrange equation must be used:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(\frac{\partial f}{\partial y'}\right) - \frac{\partial f}{\partial y} = 0$$

Hamilton's Principle of Least Action

The integral

$$S[\mathbf{q}(t)] = \int_{t_1}^{t_2} \mathcal{L}(\mathbf{q}(t), \dot{\mathbf{q}}(t), t)\mathrm{d}t$$

Is known as the **action functional**. Hamilton's Principle states that a mechanical system moves in such a way as to minimise its action.

Hamilton's Principle can written as $\delta S = 0$, where the δ represents a change with respect to the path between the end points of the integral.

The variational derivative of $\mathcal{L}$ with respect to q is the Euler-Lagrange equation.

Linear Oscillators

Equilibrium

A mechanical system that remains at rest is in equilibrium. This occurs at points in configuration space where all generalise forces $\mathcal{F}_k$ vanish.

For a conservative system, this corresponds to configurations where the potential energy $V(q_1, \ldots, q_N)$ is stationary.

Simple Harmonic Oscillator (SHO)

The Lagrangian for a simple harmonic oscillator can be written as:

$$\mathcal{L} = \frac{1}{2}m\dot{q} - \frac{1}{2}kq^2$$

$\ddot{q} + \omega^2 q = 0$ where $\omega = \sqrt{k/m}$ is a linear, homogenous differential equation and can be solved to give:

$$q(t) = q(0)\cos(\omega t) + \frac{\dot{q}(0)}{\omega}\sin(\omega t)$$

Damping Force

A frictional force F_d acts to suppress motion.

The simplest such force is

$$F_d = -\gamma\dot{q} = -\frac{m\omega}{Q}\dot{q}$$

Where Q is the dimensionless **quality factor** of the oscillator.

Damped Simple Harmonic Oscillator

The (non-conservative) damping force is incorporated into the Euler-Lagrange equation like so:

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\mathcal{L}}{\partial\dot{q}}\right) - \frac{\partial\mathcal{L}}{\partial q} = F_d$$

The result is a linear homogenous differential equation:

$$\ddot{q} + \frac{\omega}{Q}\dot{q} + \omega^2 q = 0$$

Driven Oscillators

Oscillator Driven by an External Force

Considering an undamped oscillator driven by a time-dependent external force $F(t)$ with no spatial dependence (where the driving force is not part of the dynamical system), the corresponding Lagrangian is given by:

$$\mathcal{L} = T - V = \frac{m\dot{q}^2}{2} - \left[\frac{m\omega^2 q^2}{2} - F(t)q\right]$$

Which yields the second order linear inhomogenous differential equation:

$$\ddot{q} + \omega^2 q = \frac{F(t)}{m}$$

Dirac δ-functions

To express an **impulsive force** mathematically we use Dirac δ-functions.

The effect of $\delta(t - t')$ is defined as:

$$f(t') = \int_{-\infty}^{\infty}\delta(t - t')f(t)\mathrm{d}t$$

Where $\delta(t - t')$ has units of inverse time. We can define a single impulsive force at time t' as

$$F(t) = K\delta(t - t')$$

Where K is the total impulse provided.

Response of an Oscillator to a q-Independent Impulsive Force

With $F(t) = K\delta(t - t')$, integrating the differential equation for the driven oscillator around $t = t'$ yields:

$$\int_{t'-\epsilon}^{t'+\epsilon} (\ddot{q} + \omega^2 q)\mathrm{d}t = \int_{t'-\epsilon}^{t'+\epsilon} \frac{K}{m}\delta(t-t')\mathrm{d}t$$

$$\Rightarrow \dot{q}(t'+\epsilon) - \dot{q} + \omega^2 \int_{t'-\epsilon}^{t'+\epsilon} q(t)\mathrm{d}t = \frac{K}{m}$$

Where the integral in blue tends to zero as $\epsilon \to 0$ unless $q(t') \to \infty$.

Hence there is an instantaneous change in the velocity:

$$\dot{q}(t'_+) = \dot{q}(t'_-) + \frac{K}{m}$$

Where

$$t'_\pm = \lim_{\epsilon \to 0}(t' \pm \epsilon)$$

Note that for a finite velocity:

$$q(t'_+) = q(t'_-)$$

i.e. there is no instantaneous change in position.

Time-Evolution Sequence of an SHO with an Impulsive Force

1. $t < t'$: ($F(t) = 0$) system evolves as an SHO to position $q(t'_-)$, velocity $\dot{q}(t'_-)$
2. $t = t'$: ($F(t) \neq 0$) instantaneous jump in velocity
3. $t > t'$: ($F(t) = 0$) system evolves as an SHO:

$$q(t) = q(t'_-)\cos(\omega[t-t']) + \frac{\dot{q}(t'_-) + K/m}{\omega}\sin(\omega[t-t'])$$

Causal Green's Function G

The Green's function for this system is the solution to the differential equation:

$$\ddot{G}(t-t') + \omega^2 G(t-t') = \delta(t-t')$$

And represents the response of the oscillator to a single unit-sized impulsive force, scaled as

$$G(t-t') = q(t)\frac{m}{K}$$

So that the differential equation only has a δ-function on the right-hand side.

Considering the oscillator to be at rest prior to the application of the impulsive force, the solution for G is:

For $t - t' \leq 0$:

$$G(t-t') = 0$$

For $t - t' \geq 0$:

$$G(t-t') = \frac{1}{\omega}\sin(\omega[t-t'])$$

General Driving Force $F(t)$

Using the definition of the δ-function, the equation of motion for the driven oscillator can be written as:

$$\ddot{q} + \omega^2 q = \frac{1}{m}\int_{-\infty}^{\infty} \mathrm{d}t'\ F(t')\delta(t-t')$$

Substituting in the differential equation for the Green's function G:

$$\ddot{q} + \omega^2 q = \frac{1}{m}\int_{-\infty}^{\infty} \mathrm{d}t'\ F(t')[\ddot{G}(t-t') + \omega^2 G(t-t')]$$

Which can be written as:

$$\ddot{q} + \omega^2 q = \frac{1}{m}\int_{-\infty}^{\infty} \mathrm{d}t'\ F(t')\ddot{G}(t-t') + \omega^2 \frac{1}{m}\int_{-\infty}^{\infty} \mathrm{d}t'\ F(t')G(t-t')$$

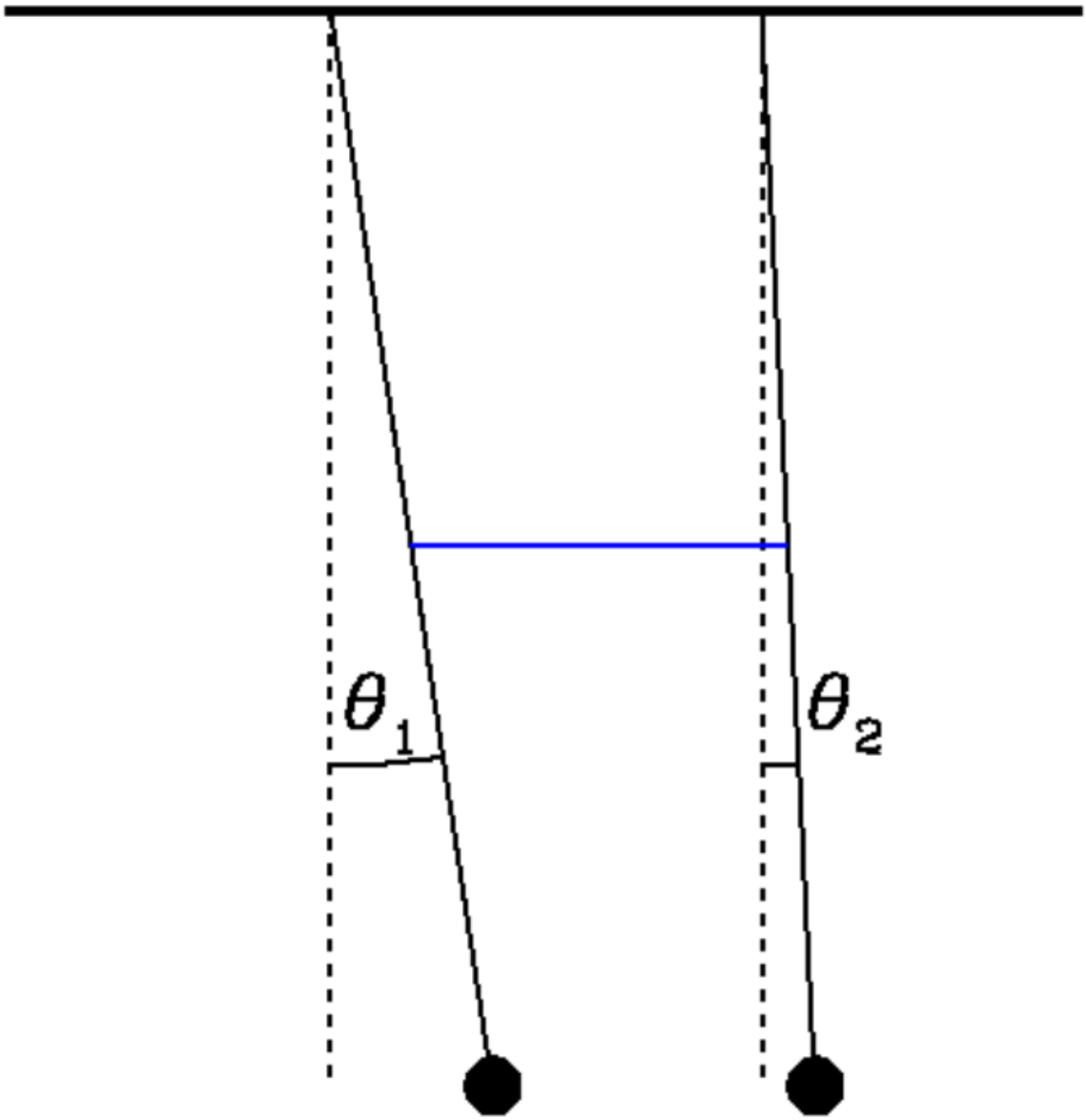
Comparing terms and substituting in the solution for $G(t-t')$ gives:

$$q(t) = \frac{1}{m}\int_{-\infty}^{t} F(t')G(t-t')\mathrm{d}t' = \frac{1}{m\omega}\int_{-\infty}^{t} F(t')\sin(\omega[t-t'])\mathrm{d}t'$$

Hence, the displacement at time t is found by summing over the displacements caused by all the preceding impulsive forces.

Coupled Small Oscillations

Two Coupled Pendulums



Consider a system with two pendula of length l connected half-way down by a spring with constant k and unstretched length equal to the horizontal separation of the pivot points.

There are two DoF with θ_1 and θ_2 as generalised coordinates. If the rigid pendula have all of their mass, m, contained in the bob and the spring is massless, then the kinetic energy is:

$$T = \frac{ml^2}{2}(\dot{\theta}_1^2 + \dot{\theta}_2^2)$$

Without coupling and assuming small oscillations:

$$V = \frac{mgl}{2}(\theta_1^2 + \theta_2^2)$$

The spring's coupling potential is:

$$V_{\text{coupling}} = \frac{k}{2}\left(\frac{l}{2}\right)^2(\theta_2 - \theta_1)^2$$

Hence

$$\mathcal{L} = \frac{ml^2}{2}(\dot{\theta}_1^2 + \dot{\theta}_2^2) - \frac{1}{2}\left(mgl(\theta_1^2 + \theta_2^2) + k\left(\frac{l}{2}\right)^2(\theta_2 - \theta_1)^2\right)$$

To remove the $\theta_1\theta_2$ cross-term, transform to **centre of mass** $\theta_c = (\theta_1 + \theta_2)/2$ and **relative** $\theta_r = \theta_2 - \theta_1$ **coordinates**.

Defining $\omega_0 = \sqrt{g/l}$ and the coupling constant $\eta = kl/(4mg)$:

$$\mathcal{L} = ml^2\left[\left(\dot{\theta}_c^2 - \omega_0^2\theta_c^2\right) + \frac{1}{4}\left(\dot{\theta}_r^2 - \omega_0^2(1+2\eta)\theta_r^2\right)\right]$$

The Euler-Lagrange equations yield two separated harmonic oscillator EoMs:

$$\ddot{\theta}_c + \omega_0^2\theta_c = 0$$

And:

$$\ddot{\theta}_r + \omega_0^2(1+2\eta)\theta_r = 0$$

A More General Recipe

1. Find an equilibrium configuration, i.e. vales of the generalised coordinates where all generalised forces $\mathcal{F}_k = -\partial V/\partial q_k = 0$
2. Taylor expand the Lagrangian $\mathcal{L}$ to second order in the generalised coordinates and velocities, around values for the generalised coordinates q_k given by the equilibrium configuration, with the values of the generalised velocities $\dot{q}_k = 0$
3. For N DoF, the Taylor expansion must in principal be in $2N$ variables.

Matrix Form of $\mathcal{L}$

If a_k are the equilibrium values of an initially used set of generalised coordinates q'_k then a new set of generalised coordinates $q_k = q'_k - a_k$ can be defined.

These q_k will have equilibrium values $= 0$ and $\mathcal{L}$ can take the form:

$$\mathcal{L} = T - V = \dot{\mathbf{q}}^T\hat{\tau}\dot{\mathbf{q}} - \mathbf{q}^T\hat{v}\mathbf{q} + c$$

Where c is a constant, $\mathbf{q}$ is a column vector and its transpose $\mathbf{q}^T = (q_1, \ldots, q_N)$ is a row vector.

The matrices $\hat{\tau}$ and $\hat{v}$ are symmetric with matrix elements given by:

$$\tau_{jk} = \frac{1}{2}\frac{\partial^2 T}{\partial\dot{q}_j\partial\dot{q}_k}\bigg|_{\dot{q}_j,\dot{q}_k=0}$$

$$v_{jk} = \frac{1}{2}\frac{\partial^2 V}{\partial q_j\partial q_k}\bigg|_{q_j,q_k=0}$$

Equations of Motion

Note that partial differentiation of the Lagrangian $\mathcal{L}$ with respect to the generalised coordinates and velocities yields:

$$\frac{\partial \mathcal{L}}{\partial \dot{q}_j} = 2\sum_{k=1}^{N} \tau_{jk}\dot{q}_k = 2(\hat{\tau}\dot{\mathbf{q}})_j$$

$$\frac{\partial \mathcal{L}}{\partial q_j} = -2\sum_{k=1}^{N} v_{jk}q_k = -2(\hat{v}\mathbf{q})_j$$

The E-L equations therefore yield:

$$\hat{\tau}\ddot{\mathbf{q}} + \hat{v}\mathbf{q} = 0$$

Normal Modes

Working Towards a Solution

Inserting a trial solution $\mathbf{q} = \mathbf{b}e^{i\omega t}$ into the Euler-Lagrange equations yield:

$$(\hat{v} - \omega^2\hat{\tau})\mathbf{b} = 0$$

We also know that unless $\mathbf{b} = 0$, this can only be fulfilled if

$$\left|-\hat{\tau}\omega^2 + \hat{v}\right| = 0$$

Calculating the determinant will yield an Nth order polynomial in ω^2. Hence there are N generalised (eigen)values of ω_j^2 each with a corresponding (eigen)vector $\mathbf{b}_j$.

Normal Coordinates

It is common to normalise the mode vectors $\mathbf{b}_{(j)}$, i.e. to have $\mathbf{b}_{(j)}^T = (b_{(j)1}, b_{(j)2}, \ldots, b_{(j)N})$ such that $\sqrt{\sum_{k=1}^{N} b_{(j)k}^2} = 1$

Using the vector elements, we may define a new set of separated generalised normal coordinates r_j via

$$r_j = \sum_{k=1}^{N} b_{(j)k}q_k$$

Note that for the couple pendulum example, $r_1 \propto (\theta_1 + \theta_2)$ and $r_2 \propto (\theta_2 - \theta_1)$.

If $\omega_j^2 > 0$, the equilibrium configuration is **stable** and the normal coordinate r_j evolves as:

$$r_j(t) = r_j(0)\cos(\omega_j t) + \frac{\dot{r}_j}{\omega_j}\sin(\omega_j t)$$

Such motion is called a **normal mode** where all parts of the system oscillate with the same frequency. Motion in general can be described by a superposition of normal modes.

If $\omega_j^2 < 0$, the equilibrium is **unstable**, and if $\omega_j^2 = 0$, the motion is also **not oscillatory**, usually corresponding to rotation or translation of the CoM.

Mode Orthogonality

As we have have been finding eigenvectors of a real symmetric matrix, they will be orthogonal i.e.:

$$\mathbf{b}_i^T\hat{\tau}\mathbf{b}_j = 0 \quad \text{if} \quad i \neq j$$

1. If ω_is are all different, then $\mathbf{b}_i$s are all unique
2. If some ω_is are the same, then there is a choice of $\mathbf{b}_i$s but we can always find orthogonal $\mathbf{b}_i$s

The $\mathbf{b}_i$s are the **natural axes** in N-dimensional space. With respect to them, the transformed potential energy, $\hat{v}'$ is diagonal. In these coordinates, the system undergoes SHO.

Central Forces

Two Interacting Bodies

Consider two bodies (with position vectors $\mathbf{r}_1$ and $\mathbf{r}_2$) interacting via a central force, defined as a force depending only on the distance r between the two bodies, directed along the line between them.

The potential energy V_{12} from which such a force is derived is only dependent on r i,e. $V_{12} = V_{12}(\mathbf{r}_1, \mathbf{r}_2) = V_{12}(|\mathbf{r}_1 - \mathbf{r}_2|) = V(r)$ for such a force.

Considering the general case of two point masses interacting via a central force, with additional external forces, then the Lagrangian is given by:

$$\mathcal{L} = \frac{1}{2}(m_1\dot{\mathbf{r}}_1^2 + m_2\dot{\mathbf{r}}_2^2) - V_1(\mathbf{r}_1) - V_2(\mathbf{r}_2) - V_{12}(|\mathbf{r}_1 - \mathbf{r}_2|)$$

Where the potentials in blue are the **external potentials** and the potential in red is the the **interaction potential**.

Ignorable Centre of Mass Motion and Conservation of Momentum

Conservation of the total momentum $\mathbf{P}$ implies that the CoM (coordinate $\mathbf{R} = (m_1\mathbf{r}_1 + m_2\mathbf{r}_2)/(m_1 + m_2)$) moves like a free particle.

Rewriting $\mathcal{L}$ in terms of $\mathbf{R}$ and the relative coordinate $\mathbf{r} = \mathbf{r}_1 - \mathbf{r}_2$:

$$\mathcal{L} = \frac{1}{2}M\dot{\mathbf{R}}^2 + \frac{1}{2}\mu\dot{\mathbf{r}}^2 - V_{12}(r)$$

Where $M = m_1 + m_2$ (**total mass**) and $\mu = m_1m_2/(m_1 + m_2)$ (**reduced mass**).

$\mathbf{R}$ does not appear in the Lagrangian $\mathcal{L}$. Such coordinates are called **ignorable**. For any ignorable generalised coordinate q, it follows from the Euler-Lagrange equation that

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{\partial\mathcal{L}}{\partial\dot{q}}\right) \equiv \dot{p}_q = 0$$

And hence that $\mathbf{P}$ is conserved in this case.

Rotational Invariance and Conservation of Angular Momentum

If we transform to the centre of mass frame (comoving with the CoM), then $\mathbf{R} = \dot{\mathbf{R}} = 0$, and $\mathcal{L} = (1/2)\mu\dot{\mathbf{r}} - V_{12}(r)$. Note that $V_{12}(r)$ is dependent on distance only, not direction, and hence $\mathcal{L}$ is rotationally invariant.

In terms of spherical coordinates, we deduce that $\dot{\mathbf{r}}^2 = \dot{x}^2 + \dot{y}^2 + \dot{z}^2 = \dot{r}^2 + r^2\dot{\theta}^2 + r^2\dot{\phi}^2\sin^2\theta$. Hence:

$$\mathcal{L} = \frac{1}{2}\mu\left[\dot{r}^2 + r^2\dot{\theta}^2 + r^2\dot{\phi}^2\sin^2\theta\right] - V_{12}(r)$$

ϕ is ignorable as it does not appear in $\mathcal{L}$. Therefore:

$$p_\phi \equiv \frac{\partial\mathcal{L}}{\partial\dot{\phi}} = \mu r^2\dot{\phi}\sin^2\theta = \text{constant} \equiv J_z$$

For any choice of z axis, the angular momentum in that direction is constant. Therefore the total angular momentum, $\mathbf{J}$ is always constant (we can always choose coordinates such that the $\mathbf{J}$ lies on the z axis).

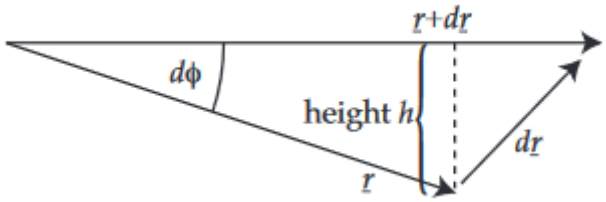
Motion Takes Place in a Plane

As $\mathbf{J} = \mathbf{r} \times \mu\dot{\mathbf{r}}$, both $\mathbf{p} \equiv \mu\dot{\mathbf{r}}$ and $\mathbf{r}$ must be perpendicular to $\mathbf{J}$.

Hence, $\mathbf{p}$ and $\mathbf{r}$ must be in a plane perpendicular to $\mathbf{J}$ and remain in that plane if $\mathbf{J}$ is to remain constant.

Choose $\mathbf{J}$ to lie along the z direction so that the angle of elevation $\theta = \pi/2, \dot{\theta} = 0$ and $J = |\mathbf{J}| = J_z = \mu r^2 \dot{\phi}$.

Equal Areas are Swept Out in Equal Times (Kepler's Second Law)



By straightforward trigonometry, the differential area $\mathrm{d}A = (1/2)|\mathbf{r} + \mathrm{d}\mathbf{r}||\mathbf{r}| \sin(\mathrm{d}\phi)$. Keeping only first-order terms, $\mathrm{d}A = (1/2)r^2 \mathrm{d}\phi$. Hence:

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{1}{2} r^2 \dot{\phi} = \frac{J}{2\mu}$$

J is conserved, so the rate at which area is swept out is constant.

Kepler's second law is therefore a consequence of angular momentum conservation and is not specific to gravity.

Equivalent 1D Problem

We can write $E = T + V = (1/2)\mu[\dot{r}^2 + r^2\dot{\theta}^2 + r^2\dot{\phi}^2 \sin^2(\theta)] + V_{12}(r)$. With $\dot{\theta} = 0, \theta = \pi/2, \dot{\phi} = J/\mu r^2$:

$$E = \frac{1}{2}\mu \dot{r}^2 + \frac{J^2}{2\mu r^2} + V_{12}(r)$$

Where the terms in blue is known as the **effective potential**, $V_{\text{eff}}(r)$, and combines the interaction potential with an **angular momentum barrier**.

The total energy E is the same as an effective Lagrangian $\mathcal{L}_{\text{eff}} = (1/2)\mu\dot{r}^2 - V_{\text{eff}}$ from which the Euler-Lagrange equation for r yields:

$$\mu \ddot{r} = \frac{J^2}{\mu r^3} - \frac{\partial V_{12}}{\partial r}$$

Gravitational Attraction

Gravitational Interaction Potential

The potential energy between two gravitating bodies of masses m_1 and m_2 is $V_{12}(r) = -k/r$ where $k = Gm_1m_2$. The differential equation to be solved is then:

$$\mu \ddot{r} = \frac{J^2}{\mu r^3} - \frac{k}{r^2}$$

Elliptical Orbits (Kepler's First Law)

Define $p \equiv J^2/\mu k$ and $\epsilon \equiv pB$. Then putting the solution for u into eqn 19 (see Eke's notes) yields:

$$E = \frac{\mu k^2}{2J^2}(\epsilon^2 - 1) = \frac{k}{2p}(\epsilon^2 - 1)$$

If $0 \leq \epsilon < 1$, the energy E is negative, implying a **bound state**. The solution to eqn 20 (see Eke's notes) can be written as:

$$p = r_\epsilon r \cos\phi$$

Expressed in cartesian coordinates, this becomes $p = \sqrt{x^2 + y^2} + \epsilon x$, or equivalently

$$(1 - \epsilon^2)x^2 + 2\epsilon p x + y^2 - p^2 = 0$$

Restricting ourselves to $0 \leq \epsilon < 1$, this above equation describes an ellipse (Kepler's first law):

$$\frac{1}{a^2}\left(x + \frac{\epsilon p}{1 - \epsilon^2}\right)^2 + \frac{y^2}{b^2} = 1$$

Where the semimajor axis $a = p/(1 - \epsilon^2)$ and the semi-minor axis $b = p/\sqrt{1 - \epsilon^2}$. The energy then takes the form $E = -k/2a$.

ϵ is the eccentricity of the elliptical orbit. $\epsilon = 0$ for a circular orbit, $\epsilon = 1$ describes a parabolic trajectory and $\epsilon > 1$ for a hyperbola.

Kepler's Third Law

From Kepler's second law, $\mathrm{d}A/\mathrm{d}t = J/(2\mu)$. The period τ of an elliptical orbit follows from the total area $A = \piab$ of that orbit, i.e., $\tau = A2\mu/J$. From this can be found that:

$$\tau = 2\pi\sqrt{\frac{1}{G(m_1 + m_2)}}a^{3/2}$$

Kepler's third law states that $\tau^2 \propto a^3$ with the same proportionality constant for all the planets. Since $M_\odot \gg M_{\text{planet}}$ this is approximately true.

Solving 1D Systems by Quadrature

Consider a 1D system such as a point mass in an external potential. The Lagrangian $\mathcal{L} = (1/2)m\dot{q}^2 - V(q)$ and it has energy $E = (1/2)m\dot{q}^2 + V(q)$. This implies:

$$\dot{q} \equiv \frac{\mathrm{d}q}{\mathrm{d}t} = \pm\sqrt{\frac{2[E - V(q)]}{m}} \implies \mathrm{d}t = \mathrm{d}q\left\{\pm\sqrt{\frac{m}{2[E - V(q)]}}\right\}$$

The time taken to move from $q = 0$ to $q(t)$ is then:

$$t = \sqrt{\frac{m}{2}}\int_0^q \mathrm{d}q'\sqrt{\frac{1}{E - V(q')}}$$

The elapsed time as a function of the coordinate $t(q)$ must be inverted to obtain $q(t)$. A problem solved as an integral is said to **solved by quadrature**.

Noether's Theorem and Hamiltonian Mechanics

Noether's Theorem

If the Lagrangian is invariant under a continuous symmetry transformation, then there are conserved quantities associated with that symmetry, one for each parameter of the transformation.

These can be found by differentiating each coordinate with respect to the parameters of the transformation in the immediate neighbourhood of the identity transformation, multiplying by the conjugate momentum, and summing over the degrees of freedom.

For example, take a point mass, m, moving in free space $\mathcal{L} = (1/2)m\dot{q}^2$. For transformed coordinates $Q = q + s$, this gives:

$$\left.\frac{\mathrm{d}Q}{\mathrm{d}s}\right|_{s=0} = 1 \implies I(q) = m\dot{q}$$

Where I is a constant of the motion. For N particles, the constant of the motion is given by:

$$I(q_1,\dots,q_N,\dot{q}_1,\dots,\dot{q}_N) \equiv \sum_{k=1}^{N} p_k \left(\frac{\mathrm{d}Q_k}{\mathrm{d}s}\right)\Big|_{s=0}$$

Where p_k is the **canonically conjugate momentum** of the coordinate.

The Hamiltonian

A Legendre transformation of a time-independent, 1 DoF Lagrangian $\mathcal{L}(q,\dot{q})$ yields the **Hamiltonian**, H:

$$H(q,p) \equiv p\dot{q} - \mathcal{L}(q,\dot{q}), \quad \text{where} \quad p \equiv \frac{\partial \mathcal{L}}{\partial \dot{q}}\bigg|_{\text{constant q}}$$

Differentiating this equation and using the Euler-Lagrange equation, we find **Hamilton's equations**:

$$\frac{\partial H}{\partial p}\bigg|_q = \dot{q}, \qquad \frac{\partial H}{\partial q}\bigg|_p = -\frac{\partial \mathcal{L}}{\partial q}\bigg|_{\dot{q}} = -\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial \mathcal{L}}{\partial \dot{q}}\bigg|_q = -\dot{p}$$

Hamilton's Equations of Motion

For N DoF, the Hamiltonian is defined using the Legendre transformation:

$$H \equiv \left(\sum_{k=1}^{N} p_k \dot{q}_k\right) - \mathcal{L}$$

Where $\mathcal{L}$ may now be now be explicitly time dependent. We can also consider time as a passive variable in the Legendre transformation, which yields:

$$\frac{\partial H}{\partial t}\bigg|_{q_1,\dots,p_1,\dots} = -\frac{\partial \mathcal{L}}{\partial t}\bigg|_{q_1,\dots,p_1,\dots} \implies \frac{\mathrm{d}H}{\mathrm{d}t} = \frac{\partial H}{\partial t} = -\frac{\partial \mathcal{L}}{\partial t}$$

If there is no explicit time dependence in $\mathcal{L}$, H is a constant of the motion.

If T is also a quadratic form in the $\dot{q}_k$, H is the total energy $E = T + V$.

Finally, **Hamilton's equations of motion** in complete generality are:

$$\dot{q}_k = \frac{\partial H}{\partial p_k}, \quad \dot{p}_k = -\frac{\partial H}{\partial q_k}, \quad \frac{\mathrm{d}H}{\mathrm{d}t} - \frac{\partial \mathcal{L}}{\partial t}$$

Canonical Transformations and Poisson Brackets

Canonical Transformations

Coordinate transformation take place in configuration space. In **phase space** one can consider new coordinates Q and momenta P that are functions of the original coordinates q, their momenta p and time t:

$$Q = Q(q,p,t), \quad P = P(q,p,t)$$

These are commonly called **contact transformations**.

A transformation is by definition canonical, if it preserves the structure of Hamilton's equations for all dynamical system.

The Generating Function

$F(q,Q,t)$ is called a **generating function**. From the chain rule, the time derivative for the generating function is:

$$\frac{\mathrm{d}F}{\mathrm{d}t} = \frac{\partial F}{\partial q}\dot{q} + \frac{\partial F}{\partial Q}\dot{Q} + \frac{\partial F}{\partial t}$$

By construction, $\dot{q}$ does not appear explicitly in $\mathcal{L}'$ (transformed Lagrangian), and so:

$$0 = \frac{\partial \mathcal{L}'}{\partial \dot{q}} = \frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial}{\partial \dot{q}}\left(\frac{\partial F}{\partial q}\dot{q} + \frac{\partial F}{\partial Q}\dot{Q} + \frac{\partial F}{\partial t}\right) = \frac{\partial \mathcal{L}}{\partial \dot{q}} - \frac{\partial F}{\partial q} \implies p = \frac{\partial F}{\partial q}$$

Similarly

$$\frac{\partial \mathcal{L}'}{\partial \dot{Q}} = -\frac{\partial F}{\partial Q} \implies P = -\frac{\partial F}{\partial Q}$$

These are known as the **implicit transformation equations**.

The Transformed Hamiltonian

To find the new Hamiltonian $H'(Q,P)$, return to the definition of H' in terms of a Legendre transformation. Hence,

$$\begin{aligned} H'(Q,P,t) &\equiv P\dot{Q} - \mathcal{L}' = -\frac{\partial F}{\partial Q}\dot{Q} - \mathcal{L} + \frac{\partial F}{\partial q}\dot{q} + \frac{\partial F}{\partial Q}\dot{Q} + \frac{\partial F}{\partial t} \\ &= p\dot{q} - \mathcal{L} + \frac{\partial F}{\partial t} \\ &= H(q,p,t) + \frac{\partial F(q,Q,t)}{\partial t} \end{aligned}$$

Poisson Brackets

For N DoF, a **Poisson bracket** for two arbitrary functions F and G is defined as:

$$\{F,G\} \equiv \sum_{k=1}^{N}\left(\frac{\partial F}{\partial q_k}\frac{\partial G}{\partial p_k} - \frac{\partial F}{\partial p_k}\frac{\partial G}{\partial q_k}\right)$$

For the case where $N = 1$:

$$\{F,G\} \equiv \frac{\partial F}{\partial q}\frac{\partial G}{\partial p} - \frac{\partial F}{\partial p}\frac{\partial G}{\partial q}$$

Clearly, $\{q,p\} = 1$. The value of the Poisson bracket for q and p is independent of the representation,

Conversely, $\{Q,P\} = 1$ is a necessary and sufficient condition for a transformation to be canonical.

Poisson Bracket Formulation of Hamilton's Equations

Hamilton's equations of motion can be reformulated in terms of Poisson brackets:

$$\dot{q} = \{q,H\}, \quad \dot{p} = \{p,H\}$$

For an arbitrary function $F(q,p,t)$:

$$\dot{F} = \{F,H\} + \frac{\partial F}{\partial t}$$

Rotating Reference Frames

Accelerating Reference Frames

One can only specify the position $\mathbf{r}_S$ or a point mass with respect to a chosen **reference frame** S. One can equally choose another reference frame B to specify the position $\mathbf{r}_B$ of the same point mass, displaced by $\mathbf{R}$ from S. The positions of the point mass relative to the two frames are then related by $\mathbf{r}_B = \mathbf{r}_S - \mathbf{R}$.

If S is an inertial frame where Newton's laws hold, but $\ddot{\mathbf{R}} \neq 0$, then B is not an inertial frame and hence in frame S, $m\ddot{\mathbf{r}}_S = \mathbf{F}$ but in frame B,

$$m\ddot{\mathbf{r}}_B = m(\ddot{\mathbf{r}}_S - \ddot{\mathbf{R}}) = \mathbf{F} - m\ddot{\mathbf{R}}$$

Where the term in blue is the **true force** and the term in red is the **fictitious force**.

Infinitesimal Rotations

Consider a point fixed in frame S at $\mathbf{r}_S = \mathbf{r}$. If frame B is infinitesimally rotated with respect to S by $\mathrm{d}\theta$, then $\mathbf{r}_B = \mathbf{r} + \mathrm{d}\mathbf{r} \quad (\implies \mathrm{d}\mathbf{r} = \mathbf{r}_B - \mathbf{r}_S)$. In the small-angle limit, the rotation formula transforms to $\mathbf{r} + \mathrm{d}\mathbf{r} = \mathbf{r} + (\mathbf{r} \times \mathbf{n})\mathrm{d}\theta$.

Hence, the velocity of the point in reference frame B relative to that in frame S is given by:

$$\left[\frac{\mathrm{d}\mathbf{r}}{\mathrm{d}t}\right]_{\text{in } B} = -\left(\mathbf{n}\frac{\mathrm{d}\theta}{\mathrm{d}t}\right) \times \mathbf{r} = -\boldsymbol{\omega} \times \mathbf{r}$$

Where $\boldsymbol{\omega}$ is the angular velocity.

Inertial Forces in a Rotating Frame

We find that:

$$m\ddot{\mathbf{r}} = \mathbf{F} - 2m\boldsymbol{\omega} \times \dot{\mathbf{r}} - m\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r}) - m\dot{\boldsymbol{\omega}} \times \mathbf{r}$$

Where the blue term is the **Coriolis force**, the red term is the **centrifugal force** and the green term is the **Euler force**.

Inertial Forces on Earth

Centrifugal Force $-m\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r})$

The direction of the centrifugal force points directly away from the axis of rotation meaning it can **counteract gravity**.

Coriolis Force $-2m\boldsymbol{\omega} \times \dot{\mathbf{r}}$

In the local coordinate system define for the surface of the Earth, the Coriolis force is given by:

$$-2m\boldsymbol{\omega} \times \dot{\mathbf{r}}' = -2m\omega(\dot{z}\sin\theta - \dot{y}\cos\theta, \dot{x}\cos\theta, \dot{x}\sin\theta)$$

Note that it is proportional to velocities and therefore only comes into play when there is motion.

Loose Ends

The Euler force is not zero on Earth but it commonly taken to be negligible.

The general EOM is given by:

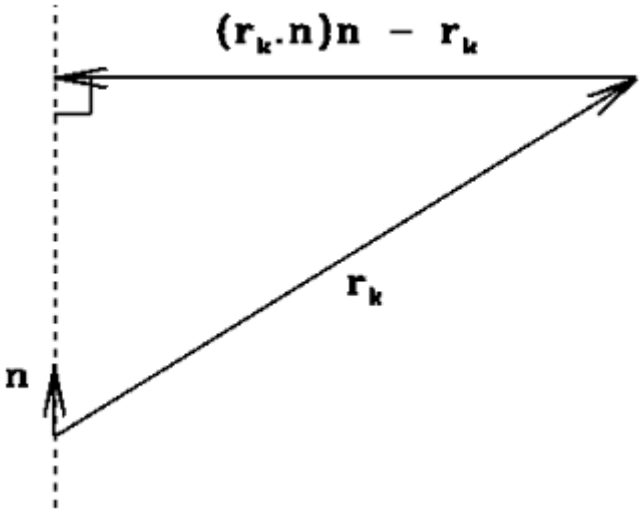
$$m\ddot{\mathbf{r}} = \mathbf{F} - 2m\boldsymbol{\omega} \times \dot{\mathbf{r}} - m\boldsymbol{\omega} \times (\boldsymbol{\omega} \times \mathbf{r}) - m\dot{\boldsymbol{\omega}} \times \mathbf{r} - m\ddot{\mathbf{R}}$$

Rotational Inertia, Angular Momentum and Kinetic Energy

DoF of Rigid Bodies

Any rigid body more complex than two connected point masses has 6 DoF. These correspond to a translation and a rotation.

Moment of Inertia I about an Axis of Rotation



Consider N mass points, rotating with angular velocity ω anticlockwise about an axis of rotation (assumed to pass through the origin), where the direction of the axis of rotation is defined by the unit vector $\mathbf{n}$.

Each mass point has moment of inertia that is the square of its distance from the axis of rotation multiplied by its mass m. For N mass points, I is the sum of such terms. Hence:

$$I = \sum_{k=1}^{N} m_k |(\mathbf{r}_k \cdot \mathbf{n})\mathbf{n} - \mathbf{r}_k|^2 = \sum_{k=1}^{N} m_k \left[r_k^2 - (\mathbf{r}_k \cdot \mathbf{n})^2\right]$$

Definition of the Inertia Tensor $\hat{I}$

We infer that:

$$J_x = \sum_{k=1} \left[m_k(r_k^2 - x_k^2)\omega_x - m_k x_k y_k \omega_y - m_k x_k z_k \omega_z\right]$$

$$J_y = \sum_{k=1} \left[m_k(r_k^2 - y_k^2)\omega_y - m_k y_k x_k \omega_x - m_k y_k z_k \omega_z\right]$$

$$J_z = \sum_{k=1} \left[m_k(r_k^2 - z_k^2)\omega_z - m_k z_k x_k \omega_x - m_k z_k y_k \omega_y\right]$$

and use the linear transformation relating the angular velocity vector $\boldsymbol{\omega}$ to the angular momentum vector $\mathbf{J}$ to define the **inertia tensor** $\hat{I}$:

$$\mathbf{J} = \hat{I}\,\boldsymbol{\omega}$$

$$\begin{pmatrix} J_x \\ J_y \\ J_z \end{pmatrix} = \begin{pmatrix} I_{xx} & I_{xy} & I_{xz} \\ I_{yx} & I_{yy} & I_{yz} \\ I_{zx} & I_{zy} & I_{zz} \end{pmatrix} \begin{pmatrix} \omega_x \\ \omega_y \\ \omega_z \end{pmatrix}$$

With:

$$I_{\alpha\beta} = \sum_{k=1}^{N} m_k \left(r_k^2 \delta_{\alpha\beta} - r_{k,\alpha} r_{k,\beta}\right)$$

For continuous rigid bodies:

$$I_{\alpha\beta} = \int_{\text{volume}} \mathrm{d}x\mathrm{d}y\mathrm{d}z\; \rho(x,y,z)(r^2\delta_{\alpha\beta} - r_\alpha r_\beta)$$

Where ρ is a mass density

Centre of Mass

The centre of mass position and velocity for a system of N mass points (mass of kth point $= m_k$) are defined by:

$$\mathbf{R}_C = \frac{\sum_{k=1}^{N} m_k \mathbf{r}_k}{M}, \quad \dot{\mathbf{R}}_C = \frac{\sum_{k=1}^{N} m_k \dot{\mathbf{r}}_k}{M}$$

The Parallel and Principal Axis Theorems

Displaced Axis Theorem

The inertia tensor of a rigid body, defined with respect to rotations about the origin can be related to the inertia tensor of the same rigid body, defined with respect to rotations about its CoM, through:

$$\hat{I} = \hat{I}_{\text{CoM}} + M\hat{A}$$

Where $\hat{A}$ can be represented by a matrix, the elements of which are determined by the elements of the CoM position vector:

$$A_{\alpha\beta} = R_C^2 \delta_{\alpha\beta} - R_{C,\alpha} R_{C,\beta}$$

Parallel Axis Theorem

From the **displaced axis theorem**, the moment of inertia I about a parallel axis is:

$$I = I_{\text{CoM}} + Md^2$$

where d is the distance of the parallel axis from the axis of rotation passing through the CoM.

Symmetric Nature of the Inertia Tensor

In any representation the inertia tensor is represented by a symmetric matrix i.e. $I_{\alpha\beta} = I_{\beta\alpha}$. We say that $\hat{I}$ is a **symmetric tensor**.

Principal Axis Theorem

Since $\hat{I}$ is a symmetric tensor and is always represented by a 3×3 symmetric matrix, it has three eigenvalues. These are the **principal moments of inertia**, called I_1, I_2, I_3.

$\hat{I}$ must also have three orthonormal eigenvectors. The directions the eigenvectors point in determine the **principal axes**, labelled 1, 2 and 3.

It is always possible to find a rotated coordinate system such that the representation of $\hat{I}$ is diagonal. The diagonal elements are the principal moments of inertia, the coordinate system is set by the principal aces, and a principal moment of inertia I_k is the moment of inertia associated with rotation about the principal axis k.

Rotating the coordinate system such that the representation of $\hat{I}$ is diagonal is a **principal axis transformation**, and that this is always possible is the **principal axis theorem**.

Deducing the Principal Axes

For highly symmetric objects, it is often possible to guess a coordinate system for which all off-diagonal elements of $\hat{I}$ are $= 0$.

Prolate ellipsoids (e.g. a rugby ball) have $I_3 < I_1 = I_2$ whereas oblate ellipsoids (e.g. smartie) have $I_3 > I_1 = I_2$.

Rigid Body Dynamics and Stability

Euler's Equations of Motion

We consider N mass points subject to rigid-body constraints, and take the time derivative of the angular momentum vector to get:

$$\dot{\mathbf{J}} = \sum_{k=1}^{N} m_k(\mathbf{r}_k \times \mathbf{F}_k)$$

Which is equal to the **total torque N**.

We assume a coordinate system defined by the principal aces and thus derive **Euler's equations of motion**:

$$I_1\dot{\omega}_1 - \omega_2\omega_3(I_2 - I_3) = N_1$$

$$I_2\dot{\omega}_2 - \omega_3\omega_1(I_3 - I_1) = N_2$$

$$I_3\dot{\omega}_3 - \omega_1\omega_2(I_1 - I_2) = N_3$$

Torque-Free Motion

If there are no external torques, then we can set $N_1 = N_2 = N_3 = 0$.

$$J^2 = J_1^2 + J_2^2 + J_3^2$$

Describes a **sphere** in angular momentum space, and

$$T = \frac{J_1^2}{2I_1} + \frac{J_2^2}{2I_2} + \frac{J_3^2}{2I_3}$$

Describes an **ellipsoid**.

Where the sphere and ellipsoid intersect shows the possible trajectories for the angular momentum components $J_k = \omega_k I_k$ (due to the conservation of angular momentum and energy).

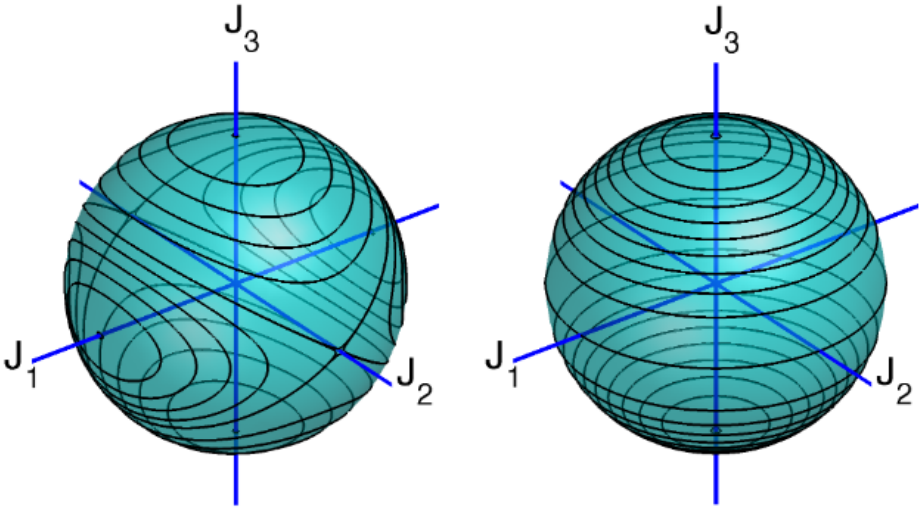


Figure 4: **Left:** Contours of constant T on a sphere described by $J^2 = 1$, for a system where $I_1 > I_2 > I_3$. Rotation about principal axis 2 is *unstable*, rotation about principal axes 1 and 3 is *stable*. **Right:** Equivalent diagram for the case where $I_1 = I_2 > I_3$. Principal axes 1 and 2 can be rotated freely about principal axis 3, and there are no points on the $J^2 = 1$ sphere about which the rotation is unstable.

Quantum Theory 2

Vector Spaces and Hilbert Spaces

Square-integrable Functions of a Real Variable

A square-integrable function of a real variable is a function $f(x)$ such that the integral

$$\int_a^b |f(x)|^2 \mathrm{d}x$$

exists and is finite or such that the integral

$$\int_{-\infty}^{\infty} |f(x)|^2 \mathrm{d}x$$

exists and is finite. Such functions also form a vector space, defining vector addition and multiplication by a scalar.

Subspaces

A subspace of a vector space V is a subset of V which itself forms a vector space under the same operations of vector addition and scalar multiplication as in V.

Linear Combinations

A linear combination of a finite number of vectors is a mathematical expression linear in the vectors involved. For example:

$$\mathbf{a} + \mathbf{b}$$

Is a linear combination of the two geometric vectors $\mathbf{a}$ and $\mathbf{b}$.

The general form of a linear combination of N vectors is:

$$c_1 v_1 + c_2 v_2 + c_3 v_3 + \cdots + c_N v_N$$

Where $v_1, v_2, v_3, \ldots, v_N$ are vectors and $c_1, c_2, c_3, \ldots, c_N$ are scalars.

The Span of a Set of Vectors

The span of a set of N vectors is the set of all linear combinations of these vectors.

Linear Independence

A set formed by N vectors $v_1, v_2, \ldots, v_N$, and these N vectors themselves, are said to be linearly independent if none of those vectors can be written as a linear combination of the other vectors of the set.

Dimension of a Vector Space

A vector space may be finite-dimensional or infinite-dimensional. A vector space is finite-dimensional and has a dimension N if it contains a linearly independent set of N vectors but no linearly independent set of more than N vectors.

It is infinite-dimensional if it contains an arbitrarily large set of linearly independent vectors.

A vector space spanned by N linearly independent vectors is finite-dimensional and its dimension is N.

Bases

A basis of a finite-dimensional vector space is a set of linearly independent vectors such that any vector belonging to this vector space can be written as linear combination of these basis vectors.

Inner Product

We will denote the dot product of two geometric vectors $\mathbf{v}$ and $\mathbf{w}$ by the usual symbol $\mathbf{v} \cdot \mathbf{w}$ and the inner product of two other vectors v and w by (v, w).

Norm of a Vector

The norm of a vector v which we will represent by the symbol $||v||$ (or $|\mathbf{v}|$ for geometric vectors) is the real number defined by the following equation:

$$||v|| = \sqrt{(v, v)}$$

Orthogonal Vectors

Two vectors are said to be orthogonal is their zero. Two orthogonal unit vectors are said to be orthonormal.

Gram-Schmidt Orthogonalisation

A set of linearly vectors can always be transformed into a set of vectors orthogonal to each other by using a method known as **Gram-Schmidt Orthogonalisation**.

Suppose we want to form three vectors a', b' and c' orthogonal to each other, starting from three linearly independent non-zero vectors a, b and c.

We can decide to include one of the latter amongst our set of orthogonal vectors. For instance, let us take a' to be the vector a.

Then we form a vector b' orthogonal to a' by subtracting from b the vector a' multiple by (a', b) and divided by (a', a'):

$$b' = b - \frac{(a', b)}{(a', a')} a'$$

The vector b' so defined is always orthogonal to a' since:

$$(a', b') = (a', b) - \frac{(a', b)}{(a', a')}(a', a') = (a', b) - (a', b) = 0$$

Note that b' cannot be the zero-vector, as otherwise the vectors a and b would not be linearly independent.

We the form a vector c' orthogonal to both a' and b' by the same process:

$$c' = c - \frac{(a', c)}{(a', a')} a' - \frac{(b', c)}{(b', b')} b'$$

Hence, a', b' and c' are all orthogonal to each other.

Orthonormal Bases

Bases formed of normalised vectors orthogonal to each other are particularly convenient. SUppose that the vectors $u_1, u_1, \ldots, u_N$ form a basis. Then, for any vectors v and w there exist a set of scalars $c_1, c_2, \ldots, c_N$ and a set of scalars $d_1, d_2, \ldots, d_N$ such that;

$$v = \sum_{j=1}^{N} c_j u_j$$

and

$$w = \sum_{j=1}^{N} d_j u_j$$

Suppose further that the vectors u_j are orthonormal, i.e. that $(u_i, u_j) = \delta_{ij}$.

The coefficients c_j and d_j can then be obtained as the inner product of the respective vector with the corresponding basis vector: $c_j = (u_j, v)$ and $d_j = (u_j, w)$. Moreover:

$$(v, w) = \sum_{j=1}^{N} c_j^* d_j$$

And therefore:

$$||v||^2 = (v, v) = \sum_{j=1}^{N} |c_j|^2$$

And

$$||w||^2 = (w, w) = \sum_{j=1}^{N} |d_j|^2$$

Orthogonal Subspaces

A subspace V' of a vector space V is said to be orthogonal to another subspace V'' of V if all the vectors of V' are orthogonal to all the vectors of V''.

Hilbert Spaces

Hilbert spaces are inner product spaces which have a further mathematical property called completeness.

Inner product spaces are vector spaces in which an inner product is defined.

Operators (I)

Linear Operators

Operators are mathematical objects which transform elements of a certain vector space into elements of the same vector space. They map vectors to vectors.

An operator A is said to be linear if it fulfils the following two conditions:

1. If w is the sum of vectors v_1 and v_2, then $Aw = Av_1 + Av_2$.
2. If w is the product of a vector v by a scalar c, then $Aw = cAv$.

Exponentials of Operators

The exponential of an operator A is defined by the following equation:

$$\exp(A) = I + A + \frac{1}{2!}A^2 + \frac{1}{3!}A^3 + \cdots = \sum_{n=0}^{\infty} \frac{1}{n!}A^n$$

Note that it is only the case that $\exp(A + B) = \exp(A)\exp(B)$ when $AB = BA$.

Commutators

The commutator of two operators A and B is defined as:

$$[A, B] = AB - BA$$

If $[A, B] = 0$, the two operators are said to commute.

The Inverse of an Operator

The inverse of an operator A, denoted by A^{-1} is defined as:

$$AA^{-1} = A^{-1}A = I$$

Where for two operators, A and B,

$$(AB)^{-1} = B^{-1}A^{-1}$$

Eigenvalues and Eigenvectors

For a non-zero vector v, it is said to be the **eigenvector** of the operator A with the **eigenvalue** λ is the following is satisfied:

$$Av = \lambda v$$

If v is function rather than a vector, it is said to be an **eigenfunction** of the operator A.

Degenerate Eigenvalues

If multiple linearly independent eigenvectors belong to the same eigenvalue, the eigenvalue is said to be **degenerate**.

The Spectrum of an Operator

The set of all eigenvalues of an operator is usually called the **spectrum of that operator**.

The Adjoint of an Operator

The adjoint of an operator A is the operator $A^\dagger$ such that:

$$(v, Aw) = (w, A^\dagger v)^*$$

Quantum States and the Dirac Notation

Quantum States and Ket Vectors

Each state of a quantum state can be described by a vector belonging to a Hilbert space.

States of quantum systems can be represented using ket vectors. These do not depend on specific coordinates, only their representations in terms of wave functions do. They do not depend on the choice of basis vectors either.

The inner product of two wavefunctions is defined as:

$$\langle \psi_a | \psi_b \rangle = \int_{-\infty}^{\infty} \psi_a^*(x) \psi_b(x) \mathrm{d}x$$

Or for two vectors:

$$\langle \chi | \chi' \rangle = (\chi, \chi') = \begin{pmatrix} a^* & b^* \end{pmatrix} \begin{pmatrix} a' \\ b' \end{pmatrix}$$

The Principle of Superposition

The principle of superposition postulates that if the vectors $|\psi_a\rangle$ and $|\psi_b\rangle$ represent physically possible states of a quantum system, then any linear combination of these two vectors also represents a physically possible state of that system.

Operators (II)

Hermitian Operators

An operator $\hat{A}$ is said to be Hermitian when:

$$\langle \phi | \hat{A} | \psi \rangle = \langle \psi | \hat{A} | \phi \rangle^*$$

for any vectors $|\phi\rangle$ and $|\psi\rangle$ this operator may act on.

Real Eigenvalues and Orthogonal Eigenvectors

The eigenvalues of a Hermitian operator are **always real**.

Eigenvectors of a Hermitian operator corresponding to different eigenvalues are **always orthogonal**.

Hermitian Matrices

Matrices representing Hermitian operators are Hermitian. A Hermitian matrix is equal to its **conjugate transpose**:

$$\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} a^* & c^* \\ b^* & d^* \end{pmatrix}$$

Projectors

An operator $\hat{A}$ is said to be **idempotent** if $\hat{A}^2 = \hat{A}$.

A **projector** is an operator which **projects a vector onto another vector**. It is defined as:

$$\hat{\mathcal{P}}_\phi = |\phi\rangle\langle\phi|$$

And is used like so:

$$\hat{\mathcal{P}}_\phi|\psi\rangle = |\phi\rangle\langle\phi|\psi\rangle = \langle\phi|\psi\rangle|\phi\rangle$$

It can be shown that $\hat{\mathcal{P}}_\phi$ is idempotent:

$$\hat{\mathcal{P}}_\phi^2 = \hat{\mathcal{P}}_\phi\hat{\mathcal{P}}_\phi = |\phi\rangle\langle\phi|\phi\rangle\langle\phi| = |\phi\rangle\langle\phi| = \hat{\mathcal{P}}_\phi$$

Assuming that $\langle\phi|\phi\rangle = 1$.

The Completeness Relation

A **complete set** of vectors is a **set of vectors spanning the whole of the vector space considered**. By definition a basis set is always a complete set.

For a finite-dimensional Hilbert space of dimension N spanned by the orthonormal basis $\{|\phi_1\rangle, |\phi_2\rangle, \ldots, |\phi_N\rangle\}$, we can say:

$$|\psi\rangle = \sum_{n=1}^{N} c_n|\phi_n\rangle = \sum_{n=1}^{N}\langle\phi_n|\psi\rangle|\phi_n\rangle = \sum_{n=1}^{N}|\phi_n\rangle\langle\phi_n|\psi\rangle = \sum_{n=1}^{N}\hat{\mathcal{P}}_{\phi_n}|\psi\rangle$$

Where $\hat{\mathcal{P}}_{\phi_n} = |\phi_n\rangle\langle\phi_n|$ projects $|\psi\rangle$ onto $|\phi_n\rangle$.

Hence **the completeness relation** is given by:

$$\sum_{n=1}^{N}|\phi_n\rangle\langle\phi_n| = \hat{I}$$

Where $\hat{I}$ is the identity operator. The $|\phi_n\rangle$s must be orthonormal and form a complete set for this to hold.

Matrix Representation in a Basis of Eigenvectors

Suppose that $\{|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_N\rangle\}$ is an orthonormal basis formed by eigenvectors of a Hermitian operator $\hat{A}$. Denoting by λ_j the eigenvalue that the eigenvector $|\psi_j\rangle$ corresponds to, we have:

$$\langle\psi_i|\hat{A}|\psi_j\rangle = \lambda_j\langle\psi_i|\psi_j\rangle = \lambda_j\delta_{ij}$$

Therefore, the off-diagonal elements of the matrix representing $\hat{A}$ in that basis are all zero and the diagonal elements are the eigenvalues λ_j:

$$A = \begin{pmatrix} \lambda_1 & 0 & \ldots & 0 \\ 0 & \lambda_2 & & \vdots \\ \vdots & & \ddots & \\ 0 & \ldots & & \lambda_N \end{pmatrix}$$

Spectral Decomposition of an Operator

For a finite-dimensional Hilbert space where $\{|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_N\rangle\}$ is an orthonormal basis that spans the space, for a an operator $\hat{A}$, it can written:

$$\hat{A} = \sum_{n=1}^{N} \lambda_n |\psi_n\rangle\langle\psi_n|$$

Where λ_n are the eigenvalues of $\hat{A}$.

Eigenvalues and Eigenvectors of Commuting Operators

Consider two Hermitian operators, $\hat{A}$ and $\hat{B}$ acting in the same finite-dimensional Hilbert space.

If $\hat{A}$ and $\hat{B}$ commute and $|\psi_n\rangle$ is an eigenvector of $\hat{A}$, then the vector $\hat{B}|\psi_n\rangle$ is also an eigenvector of $\hat{A}$ corresponding to the same eigenvalue.

One can find a basis constructed from vectors which are eigenvectors both of $\hat{A}$ and of $\hat{B}$ if and only if $\hat{A}$ and $\hat{B}$ commute. i.e. there exists a basis set $\{|\psi_1\rangle, |\psi_2\rangle, \ldots, |\psi_N\rangle\}$ and scalars λ_n and μ_n, $n = 1, 2, \ldots, N$ such that:

$$\hat{A}|\psi_n\rangle = \lambda|\psi_n\rangle$$

and

$$\hat{B}|\psi_n\rangle = \mu_n|\psi_n\rangle$$

If each pair of eigenvalues (λ_n, μ_n) corresponds to a unique $|\psi_n\rangle$, one says that the operators $\hat{A}$ and $\hat{B}$ form a **complete set of commuting operators**. This means in practice that any joint eigenvector of $\hat{A}$ and $\hat{B}$ can be unambiguously defined by a pair of quantum numbers.

Bases of Eigenvectors: Infinite-dimensional Spaces

The Hamiltonian operator is Hermitian if taken as **acting in the Hilbert space of the square-integrable functions which vanish at $x = \pm a$.** It is possible to form an orthonormal basis set of eigenfunctions of that operator, such that any element $\phi(x)$ of that Hilbert space can be written in the form of an expansion on that set of eigenfunctions i,e.:

$$\phi(x) = \sum_{n=1}^{\infty} c_n \psi_n(x)$$

Measurements and Uncertainties

The Born Rule

The probability of finding the system in state $|\phi\rangle$ given that it was in state $|\psi\rangle$ just before measurement is given by the **Born rule** or **Born postulate**:

$$\Pr(|\phi\rangle; |\psi\rangle) = \frac{|\langle\phi|\psi\rangle|^2}{\langle\phi|\phi\rangle\langle\psi|\psi\rangle}$$

In the case that the state vectors are normalised, this reduces to:

$$\Pr(|\phi\rangle; |\psi\rangle) = |\langle\phi|\psi\rangle|^2$$

Dynamical Variables and Observables

Suppose that a measurement of an observable A is made on a system in the state $|\psi\rangle$, where this observable is associated with a Hermitian operator $\hat{A}$ with eigenvalues λ_n. The probability that an observable A is found to have the value λ_n is given by:

$$\Pr(\lambda_n; |\psi\rangle) = |\langle\psi_n|\psi\rangle|^2$$

Expectation Value of an Observable

If $\hat{A}$ has p distinct eigenvalues $\lambda_1, \lambda_2, \ldots, \lambda_p$ one cane show that the expectation value of the observable is:

$$\langle\psi|\hat{A}|\psi\rangle = \sum_{n=1}^{p} \lambda_n \Pr(\lambda_n; |\psi\rangle)$$

Probability Distributions

The expectation value of the random variable, A is:

$$\langle A\rangle = \sum_{n} \lambda_n \Pr(\lambda_n; |\psi\rangle)$$

And the variance:

$$(\Delta A)^2 = \sum_{n} (\lambda_n - \langle A\rangle)^2 \Pr(\lambda_n; |\psi\rangle)$$

In Dirac notation:

$$\langle A\rangle = \langle\psi|\hat{A}|\psi\rangle$$

$$(\Delta A)^2 = \langle\psi|\hat{A}^2|\psi\rangle - \langle\psi|\hat{A}|\psi\rangle^2$$

Uncertainty Relations

It can be shown that the product of the uncertainties ΔA and ΔB always obeys the following inequality:

$$(\Delta A)^2 (\Delta B)^2 \geq -\frac{1}{4}\Big(\langle\psi|[\hat{A}, \hat{B}]|\psi\rangle\Big)^2$$

Tensor Products of Hilbert Spaces

Tensor Product

For a state vector $|\psi\rangle_A$ in the Hilbert space $\mathcal{H}_A$ which represents a state of system A and a state vector $|\phi\rangle_B$ in the Hilbert space $\mathcal{H}_B$ which represents a state of system B, the tensor product of the two is given by:

$$|\eta\rangle_{AB} = |\psi\rangle_A \otimes |\phi\rangle_B = |\phi\rangle_B \otimes |\psi\rangle_A$$

Where $|\eta\rangle_{AB}$ is a state vector in the Hilbert space $\mathcal{H}_{AB}$.

Inner Products and Operators

The inner product of two vectors of $\mathcal{H}_{AB}$ is defined in terms of the inner products for $\mathcal{H}_A$ and $\mathcal{H}_B$:

$${}_{AB}\langle\eta|\eta'\rangle_{AB} = {}_A\langle\psi|\psi'\rangle_A \times {}_B\langle\phi|\phi'\rangle_B$$

Where $\times$ represents standard scalar multiplication.

Position and Momentum

Eigenfunctions of the Momentum Operator

The x-component of the momentum of a particle is associated with the operator:#

$$P = -i\hbar\frac{\partial}{\partial x}$$

For p to be an eigenvalue of P, there should exist a square-integrable function $\psi_p(x)$ such that there is a non trivial solution of the equation:

$$-i\hbar\frac{\mathrm{d}\psi_p}{\mathrm{d}x} = p\psi_p(x)$$

Such that:

$$\int_{-\infty}^{\infty} |\psi_p(x)|^2 \mathrm{d}x$$

exists and is finite.

Normalisation to a Delta Function

For continuous p, the eigenfunctions of the momentum operator can be normalised like so:

$$\int_{-\infty}^{\infty} \psi_p^*(x)\psi_{p'}(x)\mathrm{d}x = \delta(p' - p)$$

Functions $\psi_p(x)$ satisfying this equation are said to be **normalised to a delta function in momentum space**.

Probability Densities

The probability of obtaining a result between a certain value p_1 and a certain value p_2, $\Pr([p_1, p_2])$, can be written as an integral of a probability density function:

$$\Pr([p_1, p_2]) = \int_{p_1}^{p_2} \mathscr{P}(p)\mathrm{d}p$$

I.e. $\mathscr{P}(p)$ is the probability of obtaining a value of the momentum between p and $p + \mathrm{d}p$.

Suppose that the particle is in a state described by a normalized wavefunction $\psi(x)$. Here:

$$\mathscr{P}(p) = \left|\int_{-\infty}^{\infty} \psi_p^*(x)\psi(x)\mathrm{d}x\right|^2$$

Eigenfunctions of the Position Operator

The position operator, Q, is the operator which transform $\psi(x)$ into $x\psi(x)$. Like the momentum operator, the position operator has no eigenfunction in the usual sense of the word.

The Position Representation and the Momentum Representation

The wavefunction in position space $\psi(x)$ can be written in terms of the Fourier transform of the wavefunction in momentum space $\phi(p)$ and vice versa:

$$\phi(p) = \sqrt{2\pi\hbar}\int_{-\infty}^{\infty} \exp\left(-\frac{ipx}{\hbar}\right)\psi(x)\mathrm{d}x$$

$$\psi(x) = \sqrt{2\pi\hbar}\int_{-\infty}^{\infty} \exp\left(\frac{ipx}{\hbar}\right)\phi(p)\mathrm{d}p$$

The Commutator of Q and P

The commutator of the position and momentum operators is:

$$[Q, P] = i\hbar$$

Position and Momentum Operators in 3D Space

A position operator and a momentum operator can be defined for each direction of space. In particular, the operators $\hat{x}$ and $\hat{p}_x$ for the x-direction, $\hat{y}$ and $\hat{p}_y$ for the y-direction and $\hat{z}$ and $\hat{p}_z$ for the z-direction are the same operators as those denoted by $\hat{Q}$ and $\hat{P}$.

These operators obey the commutation relations:

$$[\hat{x}, \hat{p}_x] = [\hat{y}, \hat{p}_y] = [\hat{x}, \hat{p}_z] = i\hbar$$

By contrast, operators pertaining to orthogonal directions always commute with each other.

Moreover, position operators commute with position operators and momentum operators with momentum operators.

The eigenfunction $\psi_{\mathbf{k}}(\mathbf{r})$ can be normalised as:

$$\int \psi^*_{\mathbf{k}}(\mathbf{r})\psi_{\mathbf{k}'}(\mathbf{r})\mathrm{d}^3 r = \delta(\mathbf{k}' - \mathbf{k})$$

With the 3D delta function defined by the equation:

$$\delta(\mathbf{k}' - \mathbf{k}) = \delta(k'_x - k_x)\delta(k'_y - k_y)\delta(k'_z - k_z)$$

Continua of Energy Levels

For a Hamiltonian with both discrete and continuous energy levels, we find that:

$$\sum_n \psi_n(\mathbf{r})\psi^*_n(\mathbf{r}') + \int \psi_{\mathbf{k}}(\mathbf{r})\psi^*_{\mathbf{k}}(\mathbf{r}')\mathrm{d}^3 k = \delta(\mathbf{r} - \mathbf{r}')$$

Quantum Harmonic Oscillators

The Hamiltonian and the Energy Levels of a Linear Harmonic Oscillator

The Hamiltonian of a linear harmonic oscillator is given as:

$$\hat{H} = \frac{1}{2m}\hat{p}_x^2 + \frac{1}{2}m\omega^2\hat{x}^2$$

Replacing $\hat{p}_x$ and $\hat{x}$ gives us:

$$H = -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{2}m\omega^2 x^2$$

The solution to the time independent Schrodinger equation of this:

$$\hat{H}|\psi_n\rangle = E_n|\psi_n\rangle, \quad n = 0, 1, 2, \ldots$$

Have eigenenergies E_n:

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

These eigenenergies thus form a ladder of equally spaced energy levels where the bottom "rung" or ground state energy is $E_0 = h\omega/2$.

Ladder Operators

Ladder operators, a_+ and a_- act in the following on an eigenfunction of the quantum SHO:

$$|\psi_{n+1}\rangle \propto a_+|\psi_n\rangle$$

$$|\psi_{n-1}\rangle \propto a_-|\psi_n\rangle$$

Operators are related to $\hat{a}$ where $\hat{a}$ corresponds to a_- and $\hat{a}^\dagger$ corresponds to a_+.

The two operators are the important property of satisfying the following commutation relation:

$$[\hat{a}, \hat{a}^\dagger] = 1$$

Moreover, the Hamiltonian can be written as:

$$\hat{H} = \hbar\omega\left(\hat{a}^\dagger\hat{a} + \frac{1}{2}\right)$$

It can written that:

$$\hat{a}|\psi_n\rangle = \sqrt{n}|\psi_{n-1}\rangle$$

Where $\hat{a}|\psi_0\rangle = 0$. Also:

$$\hat{a}^\dagger|\psi_n\rangle = \sqrt{n+1}|\psi_{n+1}\rangle$$

We can hence define the **number operator**, $\hat{n} = \hat{a}^\dagger\hat{a}$, which is:

$$\hat{n}|\psi_n\rangle = n|\psi_n\rangle$$

These can extended to 3D with $\hat{a}_x$, $\hat{a}_y$ and $\hat{a}_z$ where orthogonal operators commute.

Unitary Transformations

Unitary Operators

An operator $\hat{U}$ is said to be unitary if it is invertible and

$$\hat{U}^\dagger = \hat{U}^{-1}$$

Therefore, if $\hat{U}$ is unitary:

$$\hat{U}^\dagger\hat{U} = \hat{I} = \hat{U}\hat{U}^\dagger$$

The eigenvalues of a unitary operator are real or complex numbers of modulus 1. Eigenvectors of a unitary operator corresponding to different eigenvalues are always orthogonal.

Unitary transformations always conserve the inner product. If $|\psi'\rangle = \hat{U}|\psi\rangle$ and $|\phi'\rangle = \hat{U}|\phi\rangle$ then:

$$\langle\phi'|\psi'\rangle = \langle\phi|\psi\rangle$$

Transformed Operators

Suppose that the vector $|\psi\rangle$ is transformed into the vector $|\eta\rangle$ by a certain operator $\hat{A}$:

$$|\eta\rangle = \hat{A}|\psi\rangle$$

Suppose further that the vectors $|\psi\rangle$ and $|\eta\rangle$ are transformed into the vector $|\psi'\rangle$ and $|\eta'\rangle$ by a certain unitary operator, $\hat{U}$:

$$|\psi'\rangle = \hat{U}|\psi\rangle$$

$$|\eta'\rangle = \hat{U}|\eta\rangle$$

Then we see that $|eta'\rangle = \hat{U}\hat{A}|\psi\rangle = \hat{U}\hat{A}\hat{U}^\dagger|\psi'\rangle$, i.e.

$$|\eta'\rangle = \hat{A}'|\psi'\rangle$$

With $\hat{A}' = \hat{U}\hat{A}\hat{U}^\dagger$.

If $\hat{A}$ is Hermitian, $\hat{A}'$ is also Hermitian.

If $[\hat{A}, \hat{B}] = \hat{C}$ then

$$[\hat{A}', \hat{B}'] = \hat{C}' = \hat{U}[\hat{A}, \hat{B}]\hat{U}^\dagger$$

$\hat{A}$ and $\hat{A}'$ have the same eigenvalues.

$\langle \phi' | \hat{A}' | \psi' \rangle = \langle \phi | \hat{A} | \psi \rangle$ for any $|\phi\rangle$, $|\psi\rangle$.

Time Evolution

The Schrodinger Equation

The time evolution of quantum states is often described by way of time-dependent wave functions, column vectors or ket vectors satisfying the Schrodinger equation e.g.:

$$i\hbar \frac{\partial \Psi}{\partial t} = H\Psi(x, y, z, t)$$

Or, in terms of the states:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} |\Psi(t)\rangle = \hat{H} |\Psi(t)\rangle$$

The inner product $\langle \Phi(t) | \Psi(t) \rangle$ is constant if $|\Phi(t)\rangle$ and $|\Psi(t)\rangle$ evolve in time according to the Schrodinger equation.

Evolution Operator

The transformation of $|\Psi(t_0)\rangle$ to $|\Psi(t)\rangle$ can be described by an operator $\hat{U}(t, t_0)$ depending on t and t_0:

$$|\Psi(t)\rangle = \hat{U}(t, t_0) |\Psi(t_0)\rangle$$

The requirement that $|\Psi(t)\rangle$ obeys the Schrodinger equation implies that:

$$i\hbar \frac{\mathrm{d}}{\mathrm{d}t} \hat{U}(t, t_0) = \hat{H} \hat{U}(t, t_0)$$

When the Hamiltonian $\hat{H}$ is time-independent, a formal solution can be written:

$$\hat{U}(t, t_0) = \exp[-i\hat{H}(t - t_0)/\hbar]$$

Note that $\hat{H}(t - t_0) = \hat{H} \cdot (t - t_0)$ and $\hat{H}$ is **not** a function of time.

The evolution operator has the following properties:

$\hat{U}(t_0, t_0) = \hat{I}$ since $|\Psi(t_0)\rangle = \hat{U}(t_0, t_0) |\Psi(t_0)\rangle$.

For any t_0, t_1 and t,

$$\hat{U}(t, t_0) = \hat{U}(t, t_1) \hat{U}(t_1, t_0)$$

In particular, $\hat{U}(t_0, t_0) = \hat{U}(t_0, t_1) \hat{U}(t_1, t_0)$, hence

$$\hat{U}(t_0, t) \hat{U}(t, t_0) = \hat{I} = \hat{U}(t, t_0) \hat{U}(t_0, t)$$

Therefore the evolution operator is invertible and:

$$\hat{U}(t_0, t) = \hat{U}^{-1}(t, t_0)$$

The evolution operator is a unitary operator hence:

$$\hat{U}^{\dagger}(t, t_0) = \hat{U}^{-1}(t, t_0)$$

Rotations and Angular Momentum

Orbital Angular Momentum

The angular momentum operator $\hat{\mathbf{L}}^2$ is defined as:

$$\hat{\mathbf{L}}^2 = \hat{\mathbf{L}} \cdot \hat{\mathbf{L}} = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

The angular momentum operators $\hat{L}_x$, $\hat{L}_y$ and $\hat{L}_z$ follow the following commutation relations:

$$[\hat{L}_x, \hat{L}_y] = i\hbar\hat{L}_z$$

$$[\hat{L}_y, \hat{L}_z] = i\hbar\hat{L}_x$$

$$[\hat{L}_z, \hat{L}_x] = i\hbar\hat{L}_y$$

And furthermore:

$$[\hat{L}_x, \hat{\mathbf{L}}^2] = [\hat{L}_y, \hat{\mathbf{L}}^2] = [\hat{L}_z, \hat{\mathbf{L}}^2] = 0$$

The operators take the following forms:

$$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

$$L_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$L_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

Spin

The spin operator is $\hat{\mathbf{S}}$ and is denoted by:

$$\hat{\mathbf{S}} = \hat{S}_x\hat{\mathbf{x}} + \hat{S}_y\hat{\mathbf{y}} + \hat{S}_z\hat{\mathbf{z}}$$

As for the orbital angular momentum:

$$[\hat{S}_x, \hat{S}_y] = i\hbar\hat{S}_z$$

$$[\hat{S}_y, \hat{S}_z] = i\hbar\hat{S}_x$$

$$[\hat{S}_z, \hat{S}_x] = i\hbar\hat{S}_y$$

And also:

$$[\hat{S}_x, \hat{\mathbf{S}}^2] = [\hat{S}_y, \hat{\mathbf{S}}^2] = [\hat{S}_z, \hat{\mathbf{S}}^2] = 0$$

With $\hat{\mathbf{S}}^2$ defined as:

$$\hat{\mathbf{S}}^2 = \hat{\mathbf{S}} \cdot \hat{\mathbf{S}} = \hat{S}_x^2 + \hat{S}_y^2 + \hat{S}_z^2$$

Spin is unrelated to position, momentum or orbital angular momentum, thus:

$$[\hat{\mathbf{r}}, \hat{\mathbf{S}}] = [\hat{\mathbf{p}}, \hat{\mathbf{S}}] = [\hat{\mathbf{L}}, \hat{\mathbf{S}}] = 0$$

Rotations and Rotation Operators

Rotations about different axes do not commute.

Passing from $\psi(x, y, z)$ to the rotated state $\psi'(x, y, z)$ is a transformation, formally:

$$\psi'(x, y, z) = R_x(\alpha)\psi(x, y, z)$$

Where $R_x(\alpha)$ is a certain operator corresponding to a rotation by an angle α about the x-axis. Note that $R_x(\alpha = 0)$ must be the identity operator. Moreover, the rotation operator for a rotation by an infinitesimal angle must differ from the identity operator only infinitesimally. I.e. there must be an operator L_x such that:

$$R_x(\mathrm{d}\alpha) = 1 - \frac{i}{\hbar}L_x\mathrm{d}\alpha$$

It follows from this that:

$$L_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

For a general quantum state $|\psi\rangle$, a rotation through an angle α about an axis $\hat{\mathbf{n}}$ can be described by:

$$|\psi'\rangle = \hat{R}_{\hat{\mathbf{n}}}|\psi\rangle$$

Infinitesimal Generators and Finite Rotations

For rotation by an infinitesimal angle $\mathrm{d}\alpha$,

$$\hat{R}_{\hat{\mathbf{n}}}(\mathrm{d}\alpha) = \hat{I} - \frac{i}{\hbar}\hat{J}_{\hat{\mathbf{n}}}\mathrm{d}\alpha$$

One says that the angular momentum operator $\hat{J}_{\hat{\mathbf{n}}}$ is the **infinitesimal generator** of the rotations about the axis $\hat{\mathbf{n}}$ in the Hilbert space of the state vectors of the system.

For a finite or infinitesimal value of α:

$$\hat{R}_{\hat{\mathbf{n}}}(\alpha) = \exp\left(-\frac{i}{\hbar}\alpha\hat{J}_{\hat{\mathbf{n}}}\right)$$

Symmetries and Conservation Laws

The expectation value of the Hamiltonian must be the same in the rotated system as in the unrotated system. In other words:

$$\langle\psi'|\hat{H}|\psi'\rangle = \langle\psi|\hat{H}|\psi\rangle$$

if the system is invariant under rotation. It is possible to deduce from this that $\hat{J}_{\hat{\mathbf{n}}}$ commutes with $\hat{H}$.

Angular Momentum Operators

The eigenvalues of $\hat{\mathbf{J}}^2$ are $j(j+1)\hbar^2$ where j is a non-negative integer $(0, 1, 2, \ldots)$ or half-integer ($1/2, 3/2, 5/2, \ldots$):

$$\hat{\mathbf{J}}^2|j,m\rangle = j(j+1)\hbar^2|j,m\rangle$$

The eigenvalues of $\hat{J}_z$ are $m\hbar$ where m is an integer $(0, \pm1, \pm2, \ldots)$ or half-integer $(\pm1/2. \pm 3/2, \pm5/2, \ldots)$. In the case of simultaneous eigenvectors of $\hat{\mathbf{J}}^2$ and $\hat{J}_z$, the possible values of j and m are restricted to be in the range $-j \leq m \leq j$, with m running from $-j$ to j by integer step. Therefore:

$$\hat{J}_z|j,m\rangle = m\hbar|j,m\rangle$$

Since eigenvectors belonging to different eigenvalues of a Hermitian operator are always orthogonal:

$$\langle j,m|j',m'\rangle = \delta_{jj'}\delta_{mm'}$$

Pauli Matrices

The matrix forms of the angular momentum operators are as follows:

$$J_x = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \quad J_y = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}, \quad J_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

Which are usually written in terms of the Pauli matrices:

$$J_x = \frac{\hbar}{2}\sigma_x, \quad J_y = \frac{\hbar}{2}\sigma_y, \quad J_z = \frac{\hbar}{2}\sigma_z$$

The Clebsch-Gordan Coefficients

Consider a system formed by two electrons, electron 1 and electron 2. Electron 1 can be, e.g. in the state of spin up, $|+\rangle_1$. Likewise electron 2 can be, e.g. in the state of spin down, $|-\rangle_2$.

In general the two-electron system can be in a join spin state represented by the ket vector:

$$|\psi\rangle_{12} = \alpha|+\rangle_1|+\rangle_2 + \beta|+\rangle_1|-\rangle_2 + \gamma|-\rangle_1|+\rangle_2 + \delta|-\rangle_1|-\rangle_2$$

Where α, β, γ and δ and four complex numbers.

More general joint angular momentum states of bipartite systems can be written in the following way:

$$|\psi\rangle_{12} = \sum_{j_1 m_1 j_2 m_2} c_{j_1 m_1 j_2 m_2} |j_1, m_1\rangle_1 |j_2, m_2\rangle_2$$

Where the kets $|j_1, m_1\rangle_1$ pertain to one part of the who system and the kets $|j_2, m_2\rangle_2$ to the other part.

Note that the angular momentum operator $\hat{\mathbf{J}}_1$ acts only on the state vectors pertaining to part 1 of the whole system while $\hat{\mathbf{J}}_2$ acts only on the state vectors pertaining to part 2.

Let $\hat{\mathbf{J}} = \hat{\mathbf{J}}_1 + \hat{\mathbf{J}}_2$. Each component of $\hat{\mathbf{J}}$ is the sum of the corresponding components of $\hat{\mathbf{J}}_1$ and $\hat{\mathbf{J}}_2$:

$$\hat{\mathbf{J}} = \hat{J}_x\hat{\mathbf{x}} + \hat{J}_y\hat{\mathbf{y}} + \hat{J}_z\hat{\mathbf{z}}$$

$$\hat{\mathbf{J}}_1 = \hat{J}_{1x}\hat{\mathbf{x}} + \hat{J}_{1y}\hat{\mathbf{y}} + \hat{J}_{1z}\hat{\mathbf{z}}$$

$$\hat{\mathbf{J}}_2 = \hat{J}_{2x}\hat{\mathbf{x}} + \hat{J}_{2y}\hat{\mathbf{y}} + \hat{J}_{2z}\hat{\mathbf{z}}$$

Where:

$$\hat{J}_z = \hat{J}_{1z} + \hat{J}_{2z}$$

It is possible to construct a basis of simultaneous eigenvectors of $\mathbf{J}_1^2$, $\mathbf{J}_2^2$, $\mathbf{J}^2$ and J_z. We will denote such simultaneous eigenvectors by $|j_1, j_2, J, M\rangle_{12}$:

$$\hat{\mathbf{J}}_1^2|j_1, j_2, J, M\rangle_{12} = j_1(j_1+1)\hbar^2|j_1, j_2, J, M\rangle_{12}$$

$$\hat{\mathbf{J}}_2^2|j_1, j_2, J, M\rangle_{12} = j_2(j_2+1)\hbar^2|j_1, j_2, J, M\rangle_{12}$$

$$\hat{\mathbf{J}}^2|j_1, j_2, J, M\rangle_{12} = J(J+1)\hbar^2|j_1, j_2, J, M\rangle_{12}$$

$$\hat{J}_z^2|j_1, j_2, J, M\rangle_{12} = M\hbar|j_1, j_2, J, M\rangle_{12}$$

For given values of j_1 and j_2, the possible values of J and M in simultaneous eigenvectors of $\mathbf{J}_1^2$, $\mathbf{J}_2^2$, $\mathbf{J}^2$ and $\mathbf{J}_z$ are restricted by the **triangular inequality**:

$$|j_1 - j_2| \leq J \leq j_1 + j_2$$

And by the usual condition that:

$$-J \leq M \leq J$$

Each of the eigenvectors $|j_1, j_2, J, M\rangle_{12}$ can be written as a linear combination of the vectors $|j_1, m_1\rangle_1|j_2, m_2\rangle_2$. The coefficients of this superposition are real numbers called the **Clebsch-Gordan coefficients**:

$$|j_1, j_2, J, M\rangle_{12} = \sum_{m_1, m_2} \langle j_1, j_2, m_1, m_2|J, M\rangle |j_1, m_1\rangle_1 |j_2, m_2\rangle_2$$

Reciprocally:

$$|j_1, m_1\rangle_1|j_2, m_2\rangle_2 = \sum_J \langle j_1, j_2, m_1, m_2|J, M\rangle |j_1, j_2, J, M\rangle_{12}$$

Where $\langle j_1, j_2, m_1, m_2 | J, M \rangle$ are the Clebsch-Gordan coefficients.