

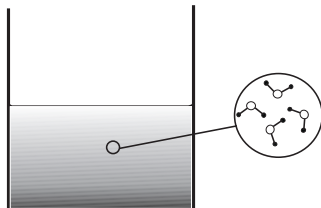
CLASSICAL MECHANICS

Michaelmas Term 2006

4 Lectures

Prof M. Brouard

Atoms and molecules



Classical versus quantum mechanics

Classical motions of small groups of isolated atoms and molecules

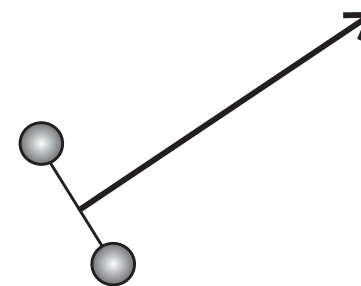
*'Theoretical chemistry is in fact physics'*¹

Richard Feynman
Lectures on Physics

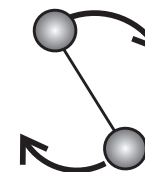
¹He also said 'Inorganic Chemistry is, as a science, now reduced to physical chemistry and quantum chemistry.'

Types of Motion (The things molecules do!)

Translation (lectures 1,2)



Rotation (lecture 3)



Vibration (lecture 4)



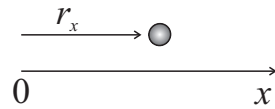
What is motion?

LECTURE 1: Translational Motion

Motion of a particle in One Dimension (along x)

Position (coordinates) [Units: m]

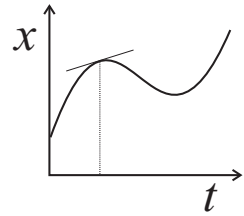
$$r_x(t)$$



Velocity

[Units: m s^{-1}]

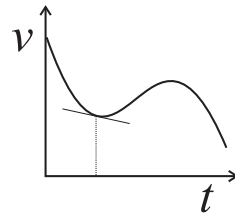
$$v_x(t) = \frac{dr_x}{dt} \equiv \dot{r}_x$$



Acceleration

[Units: m s^{-2}]

$$a_x(t) = \frac{dv_x}{dt} = \frac{d^2r_x}{dt^2} \equiv \ddot{r}_x$$



r , v and a define the motion or *trajectory* of a particle.

SEE EXAMPLES 1 AND 2

Equations of motion for constant acceleration

Acceleration

$$a_x(t) = a$$

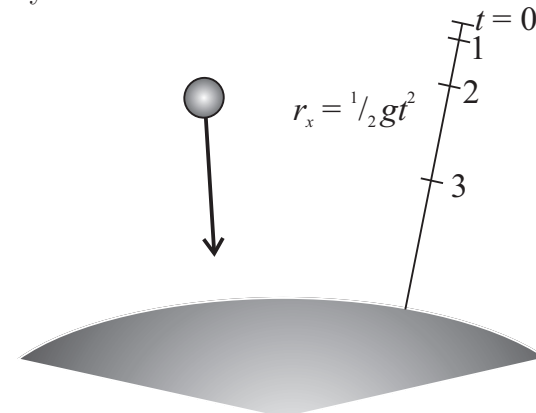
Velocity

$$v_x(t) = v_0 + at$$

Position

$$r_x(t) = r_0 + v_0t + \frac{1}{2}at^2$$

EXAMPLE: Close to the earth's surface the acceleration due to gravity, g , is approximately constant.



An Aside - Vectors

A quantity with both magnitude and direction.

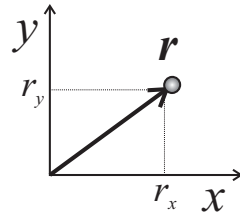
EXAMPLE (in two dimensions):

Position \mathbf{r} (of magnitude r and direction θ with respect to the x axis)

Components

$$r_x = r \cos \theta$$

$$r_y = r \sin \theta$$



Magnitude

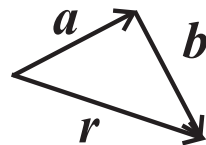
$$r = \sqrt{(r_x^2 + r_y^2)}$$

Direction

$$\tan \theta = \frac{r_y}{r_x}$$

Vector Addition²

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



i.e.

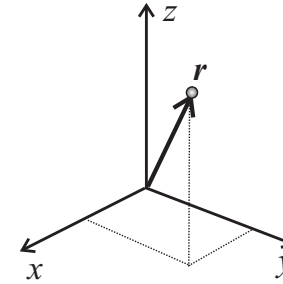
$$r_x = a_x + b_x$$

$$r_y = a_y + b_y$$

²Products of vectors may also be defined - see *Maths Course*.

Motion in three dimensions

Resolve the motion along *three Cartesian coordinates*



For **constant acceleration**

$$a_x(t) = a_x$$

$$a_y(t) = a_y$$

$$v_x(t) = v_{x0} + a_x t$$

$$v_y(t) = v_{y0} + a_y t$$

$$r_x(t) = r_{x0} + v_{x0} t + \frac{1}{2} a_x t^2$$

$$r_y(t) = r_{y0} + v_{y0} t + \frac{1}{2} a_y t^2$$

$$a_z(t) = a_z$$

$$v_z(t) = v_{z0} + a_z t$$

$$r_z(t) = r_{z0} + v_{z0} t + \frac{1}{2} a_z t^2$$

These three sets of equations can be written more neatly using *vectors* (see Aside)

$$\mathbf{a}(t) = \mathbf{a}$$

$$\mathbf{v}(t) = \mathbf{v}_0 + \mathbf{a}t$$

$$\mathbf{r}(t) = \mathbf{r}_0 + \mathbf{v}_0 t + \frac{1}{2} \mathbf{a}t^2$$

SEE EXAMPLE 3

Newton's Laws of motion

What do the laws tell us?

They enable us to *predict* the motion of particles.

1st law

Tells us what happens when we leave an object alone, i.e. in the absence of forces.

2nd Law

Tells us how to calculate the change in motion of an object if it is not left alone, i.e. how forces change motion.

3rd Law

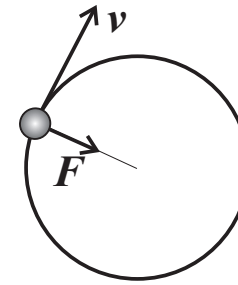
Tells us a little *about* forces and how they operate (next lecture).

Are the laws correct?

NO! But they are often a very good approximation.

1.) *Every body continues in its state of rest or uniform motion in a straight line unless it is compelled to change by forces impressed upon it.*

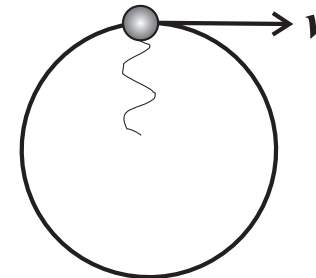
Changes in velocity (i.e. acceleration) arise from forces.



(See Lecture 3)

No force, F , implies no acceleration.

(Suggests $F \propto a$?)



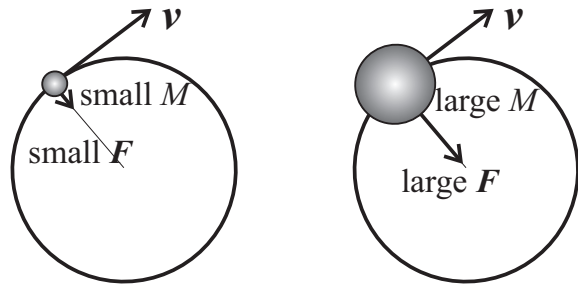
What is the relationship between force and acceleration?

Inertia and Mass

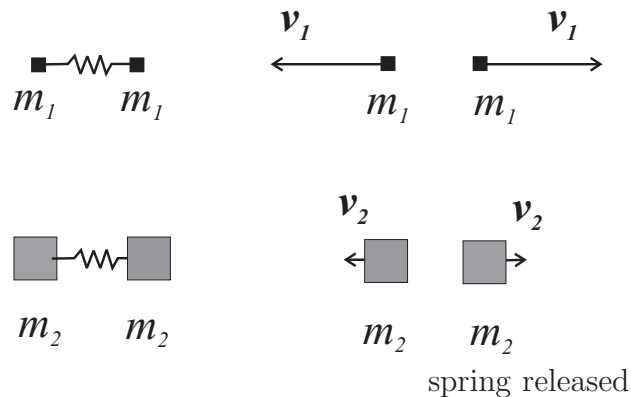
Inertia is the tendency to resist change in the state of motion.

Mass is the measure of inertia.

The mass of an object quantifies how difficult it is to change the magnitude or direction of its velocity.



Determining relative mass



2.) The force, \mathbf{F} , acting on a particle of mass m produces an acceleration $\mathbf{a} = \mathbf{F}/m$ in the direction of the force:

$$\mathbf{F} = m\mathbf{a}$$

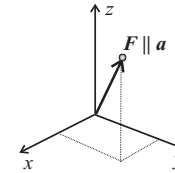
Units: $\text{N} \equiv \text{kg m s}^{-2}$

Force is a vector quantity

$$F_x = ma_x$$

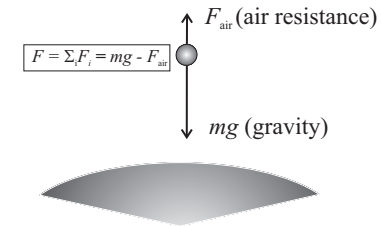
$$F_y = ma_y$$

$$F_z = ma_z$$



If more than one force, then the *net (or resultant) force*, $\sum_i \mathbf{F}_i$, determines the acceleration of the particle:

$$\sum_i \mathbf{F}_i = m\mathbf{a}$$



If we know the force we can calculate the particle's motion!

SEE EXAMPLE 4

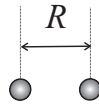
LECTURE 2: Momentum and energy conservation

Types of forces

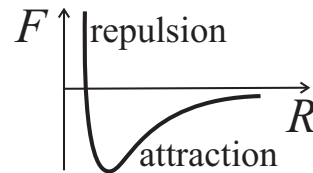
To use Newton's Laws we need to know more about the forces.

We need formulae for the forces.

Frictional Forces



Molecular Forces



Fundamental Forces (Interactions)

Interaction	Relative strength	Range	Comments
Strong	1	10^{-15} m	Holds nucleus together
Electromagnetic	10^{-2}	Infinite	Chemistry and most everyday forces
Weak	10^{-6}	10^{-17} m	Associated with radioactivity
Gravitational	10^{-38}	Infinite	Causes apples to fall on earth

The electrostatic force between an electron and a proton in the H atom exceeds gravitation by $\sim 10^{40}$!

1. Gravitation Force:

The *gravitational force* between point or spherical masses, m and M , is

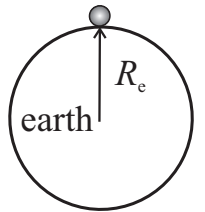
$$F = -\frac{GmM}{r^2}$$

$$G = 6.67 \times 10^{-11} \text{ N m}^2 \text{ kg}^{-2}$$

The weight, w , of an object is the net gravitational force acting on it.

For objects close to the earth's surface ($r = R_e$):

$$w = mg \quad g = \frac{GM_e}{R_e^2} \simeq 9.8 \text{ m s}^{-2}$$



where g is the acceleration due to gravity.

2. Coulomb Force:

In a vacuum, the *Coulomb force* between point or spherical charges, q and Q , is (see Electrostatics Lectures)

$$F = \frac{qQ}{4\pi\epsilon_0 r^2}$$

$$\frac{1}{4\pi\epsilon_0} = 9.0 \times 10^9 \text{ N m}^2 \text{ C}^{-2}$$

Unlike gravity (which is always attractive), the Coulomb force can be *either* attractive (< 0) or repulsive (> 0) depending on the sign of the charges.

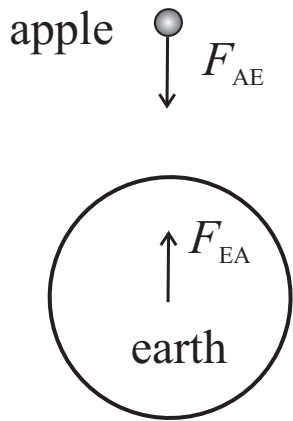
Newton's 3rd Law: A general law for the forces

3.) *The force exerted on a body A by body B is equal and opposite to the force exerted on B by A.*

$$\mathbf{F}_{AB} = -\mathbf{F}_{BA}$$

Forces act on bodies (if there is no matter there is no force).

Forces come in pairs, i.e. a force is exerted by one body on another body



$$\begin{aligned} \mathbf{F}_{AE} &= -\mathbf{F}_{EA} \\ m_A \mathbf{a}_A &= -M_E \mathbf{a}_E \\ \mathbf{a}_A &= -M_E/m_A \mathbf{a}_E \end{aligned}$$

Note that

$$\frac{M_E}{m_A} \sim 10^{24}$$

Linear Momentum

Definition

$$\mathbf{p} = m\mathbf{v}$$



Newton's Second Law (for single force \mathbf{F}) can be expressed in terms of the linear momentum :

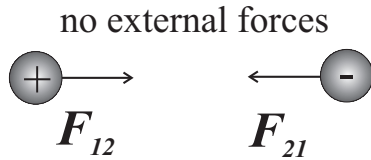
$$\mathbf{F} = m\mathbf{a} = m \frac{d\mathbf{v}}{dt} \equiv \frac{d\mathbf{p}}{dt} ,$$

where it is been assumed that the mass is time-independent. If there is no force

$$\mathbf{F} = 0 = \frac{d\mathbf{p}}{dt} \quad \text{i.e. } \mathbf{p} = \text{constant}$$

If the net force is zero the momentum is constant.

Conservation of Linear Momentum



Using Newton's 3rd Law

$$\mathbf{F}_{12} = -\mathbf{F}_{21}$$

Using Newton's 2nd Law

$$\frac{d\mathbf{p}_1}{dt} + \frac{d\mathbf{p}_2}{dt} = 0$$

Integrating

$$\Delta\mathbf{p}_1 + \Delta\mathbf{p}_2 = 0$$

where

$$\Delta\mathbf{p} = \mathbf{p}(t_2) - \mathbf{p}(t_1) .$$

This implies that

$$\mathbf{p}_1 + \mathbf{p}_2 = \text{constant}$$

If the net external force on a system is zero, the total linear momentum is constant.

SEE EXAMPLE 5

Energy and its conservation

'There is a fact, or if you wish, a law, governing all natural phenomena that are known to date. There is no known exception to this law - it is exact so far as we know. The law is called conservation of energy.'

'It states that there is a certain quantity, which we call energy, that does not change in the manifold changes which nature undergoes.'

Richard Feynman
Lectures on Physics

Kinetic Energy

Due to motion of particle

Potential Energy

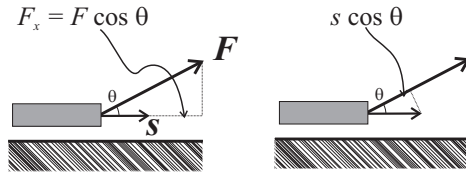
Stored energy arising from position of particle

Heat energy

Due to the kinetic energies of atoms and molecules
(see Thermodynamics)

Mechanical Work, W

Learn about energy by looking at *work*.



The *mechanical work*, W , done by a constant force, F , is

$$W = F s \cos \theta$$

Units : Joule (J) \equiv N m

where s is the total displacement, and $s \cos \theta$ is the displacement along the direction of the force.³

If the displacement *in the direction of the force* is zero, no work is done.

If the force, F_x , is *not constant*, the mechanical work is defined

$$W = \int_{x_1}^{x_2} F_x dx$$

where dx is the infinitesimal displacement along x .

³In vector notation, this equation can be written $W = \mathbf{F} \cdot \mathbf{s}$ (i.e. a scalar product of vectors).

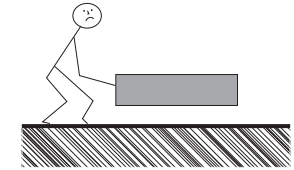
Kinetic Energy, K

The *kinetic energy*, K , of a particle is the energy a particle possesses by virtue of its motion.

For a particle of mass m moving along x with velocity v_x

$$K = \frac{1}{2} m v_x^2$$

frictionless surface



Return to the equation for the work done on a particle

$$W = \int dW = \int F_x dx$$

Use Newton's 2nd Law to rewrite $F_x dx = m v_x dv_x$

$$W = \int_{v_1}^{v_2} m v_x dv_x = \frac{1}{2} m (v_2^2 - v_1^2)$$

The work done on the particle is equal to its change in kinetic energy⁴

$$W = \Delta K$$

If an object is pushed it picks up speed

SEE EXAMPLE 6

⁴This is known as the work-energy theorem.

Potential Energy, V .

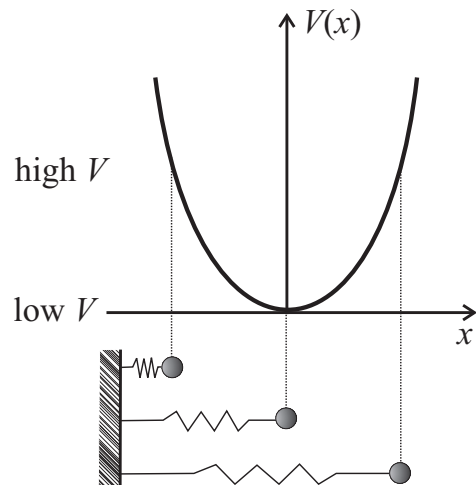
The potential energy, V , is the energy associated with the position of a particle

Potential energy may be thought of as stored energy, or the *capacity to do work*.

EXAMPLE

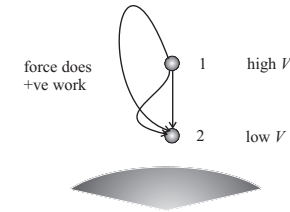
Harmonic Spring

$$V(x) = \frac{1}{2}kx^2$$



Force, work, and potential energy

For some forces⁵, the work done by the force is *independent of the path* taken.



For example, the infinitesimal work done dW by the gravitational force F is *independent of path*

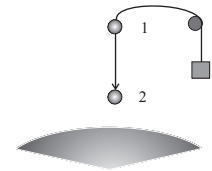
$$dW = F dx$$

In moving the particle from position 1 to 2 its capacity to do work is reduced. **The fixed amount of work is therefore *minus the change in potential energy*:**

$$dV = -dW$$

Combining these two equations yields

$$F = -\frac{dV}{dx}$$



Therefore, the (finite) *change in potential energy* between points x_1 and x_2 is

$$V(x_2) - V(x_1) = \Delta V = -\int_1^2 F_x dx = -W$$

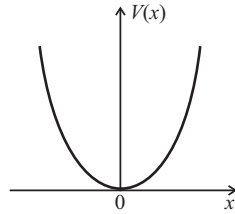
⁵They are called *conservative forces*, and include gravity and the Coulomb force. Conservative forces can be represented by potential energy functions because they depend solely on position. For non-conservative forces, such as friction, the work done and the force depends on the path taken.

EXAMPLES of potential energy functions:

Harmonic spring potential

$$V(x) = \frac{1}{2}kx^2$$

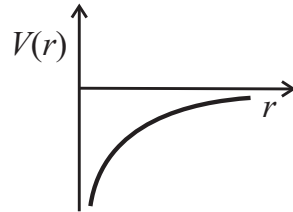
$$F(x) = -\frac{dV}{dx} = -kx$$



*Gravitational potential*⁶

$$V(r) = -\frac{GmM}{r}$$

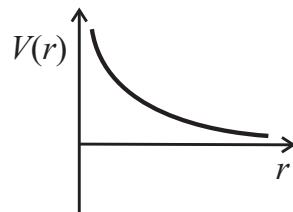
$$F(r) = -\frac{dV}{dr} = -\frac{GmM}{r^2}$$



Coulomb potential (e.g., charges q and Q of the same sign)

$$V(r) = \frac{qQ}{4\pi\epsilon_0 r}$$

$$F(r) = -\frac{dV}{dr} = \frac{qQ}{4\pi\epsilon_0 r^2}$$



⁶Close to the earth this may be approximated by

$$V(h) \simeq mgh \quad g = 9.8 \text{ m s}^{-2}.$$

*Conservation of Mechanical Energy*⁷

As shown above, the work done *by* a force is related to changes in both the kinetic and the potential energies:

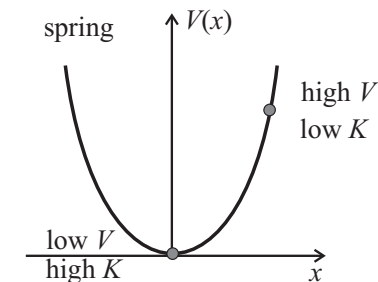
$$W = \Delta K = -\Delta V$$

Rearranging the right side of this equation yields

$$\Delta K + \Delta V = 0$$

Therefore, the sum of these energies, called the total energy, E , must be constant:

$$E = K + V$$

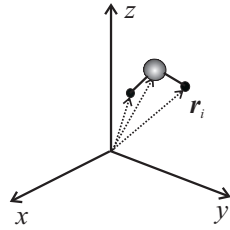


SEE EXAMPLE 7

⁷Again we focus exclusively on conservative forces, i.e. those illustrated above, which may be expressed in terms of a potential energy function.

LECTURE 3: Rotational Motion

Systems of Particles and centre-of-mass



For each particle i

$$\mathbf{F}_i = m_i \frac{d^2 \mathbf{r}_i}{dt^2}$$

where \mathbf{r}_i and m_i are the positions and masses of the constituent particles in the system.

The total force on the system is

$$\sum_i \mathbf{F}_i = \mathbf{F} = \frac{d^2(\sum_i m_i \mathbf{r}_i)}{dt^2}$$

i.e. the total force F is the *external force* acting on the system.⁸

Define a quantity, called the *centre-of-mass* (CM)

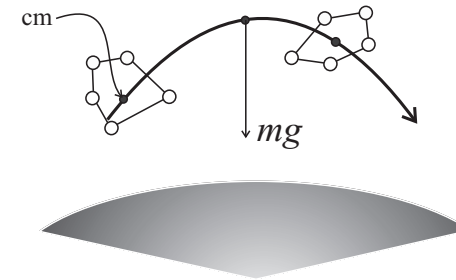
$$\mathbf{r}_{\text{CM}} = \frac{\sum m_i \mathbf{r}_i}{M}$$

where M is the total mass. Substitute into equation for \mathbf{F} yields

$$\mathbf{F} = M \frac{d^2 \mathbf{r}_{\text{CM}}}{dt^2} = M \mathbf{a}_{\text{CM}}$$

⁸This is true because all the *internal forces* between all pairs of particles in the system must cancel, because of Newton's 3rd Law.

Motion of the centre-of-mass

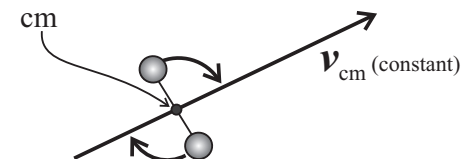


$$\mathbf{F} = M \mathbf{a}_{\text{CM}} = \frac{d\mathbf{p}_{\text{CM}}}{dt}$$

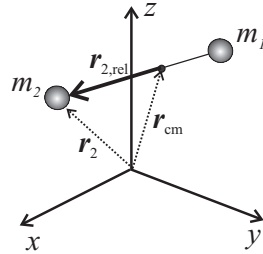
If the system of particles is isolated

$$\mathbf{F} = \frac{d\mathbf{p}_{\text{CM}}}{dt} = 0$$

If the external force on a system of particles is zero, the momentum of the centre-of-mass is constant.



Centre-of-mass and relative motion - an aside



The position of each particle, i , can be written

$$\mathbf{r}_i = \mathbf{r}_{\text{CM}} + \mathbf{r}_{i,\text{rel}} \quad (\text{vector addition})$$

Multiply through by m_i , and sum over all particles, i ,

$$\sum_i m_i \mathbf{r}_i = M \mathbf{r}_{\text{CM}} + \sum_i m_i \mathbf{r}_{i,\text{rel}}$$

But

$$\sum_i m_i \mathbf{r}_i = M \mathbf{r}_{\text{CM}}$$

Therefore

$$\sum_i m_i \mathbf{r}_{i,\text{rel}} = 0$$

Taking the time derivative of this expression yields

$$\sum_i \mathbf{p}_{i,\text{rel}} = 0$$

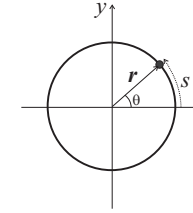
The sum of the momenta relative to the CM is zero.⁹

⁹You might also like to show that the total kinetic energy of the system can be factorized:

$$K = \sum K_i = K_{\text{CM}} + K_{\text{rel}} = \frac{1}{2} M v_{\text{CM}}^2 + \sum \frac{1}{2} m_i v_{i,\text{rel}}^2$$

where K_{CM} is the kinetic energy associated with motion of the CM and K_{rel} is the kinetic energy associated with the internal motion *relative* to the CM.

Uniform Rotation of Rigid Bodies about a Fixed Axis



The *radian*, θ , is defined by the equation

$$\theta = \frac{s}{r}$$

and the *angular velocity*, ω (units rad s^{-1}), by the equation

$$\omega = \frac{d\theta}{dt} \quad \left(\text{cf. } v = \frac{dr}{dt} \right)$$

The rotational period, T , and rotational frequency, f are related to ω by the equations

$$\omega = \frac{2\pi}{T} = 2\pi f$$

For uniform circular motion, the angular velocity is constant (i.e. zero *angular acceleration*) and one may write

$$\theta = \omega t$$

where it is assumed that at $t = 0$, $\theta = 0$. We may thus write

$$r_x = r \cos \theta = r \cos(\omega t)$$

$$r_y = r \sin \theta = r \sin(\omega t)$$

with

$$r = (r_x^2 + r_y^2)^{1/2}$$

Taking the time derivative

$$v_x = -rw \sin(\omega t)$$

$$v_y = rw \cos(\omega t)$$

i.e.

$$\mathbf{v} = \mathbf{r} \times \boldsymbol{\omega}$$

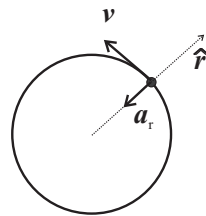
Finally, taking the time derivative a second time yields

$$a_x = -r\omega^2 \cos(\omega t)$$

$$a_y = -r\omega^2 \sin(\omega t)$$

or

$$a_r = -r\omega^2$$



In vector notation, this may be written

$$\mathbf{a}_r = -r\omega^2 \hat{\mathbf{r}} \equiv -\frac{v^2}{r} \hat{\mathbf{r}}$$

Thus, for uniform circular motion, the *centripetal acceleration* points radially inwards along $-\mathbf{r}$.

Centripetal (pointing centrally) acceleration is constant in magnitude but not in direction. The magnitude of the centripetal *force* is

$$F_r = \frac{mv^2}{r}$$

Equations of Motion (non-uniform circular motion)

If a particle experiences a **constant angular acceleration** (leading to a change in angular velocity)

$$\frac{d\omega}{dt} = \alpha \quad \text{Units } \text{rad s}^{-2}$$

then the equations of motion (from Newton's laws) can be written

$$\omega = \omega_0 + \alpha t$$

$$\theta = \theta_0 + \omega_0 t + \frac{1}{2} \alpha t^2 \quad \left(\text{cf. } r = r_0 + v_0 t + \frac{1}{2} a t^2 \right)$$

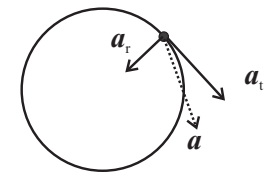
analogous to the equations for linear motion with constant linear acceleration.

In the presence of angular acceleration, the net linear acceleration can be written

$$\mathbf{a} = \mathbf{a}_r + \mathbf{a}_t$$

i.e.,

$$a = \sqrt{a_r^2 + a_t^2}$$



where the tangential (angular) acceleration, \mathbf{a}_t , is

$$\mathbf{a}_t = \boldsymbol{\alpha} \times \mathbf{r}$$

which is just the time derivative of $\mathbf{v} = \mathbf{r} \times \boldsymbol{\omega}$.

Rotational Kinetic Energy and Moments of Inertia

The kinetic energy of a particle, i , rotating with a constant angular frequency ω about a fixed axis is (using $v = r\omega$, and dropping the 'rel' on $r_{i,\text{rel}}$)

$$K_{i,\text{ang}} = \frac{1}{2}m_i v_i^2 = \frac{1}{2}m_i r_i^2 \omega^2$$

where r_i is the particle's distance from the axis of rotation.

For a system of particles all rotating with frequency ω , the rotational (angular) kinetic energy is therefore

$$K_{\text{ang}} = \sum_i K_{i,\text{ang}} = \frac{1}{2} \sum m_i r_i^2 \omega^2$$

Defining *the moment of inertia, I* , as

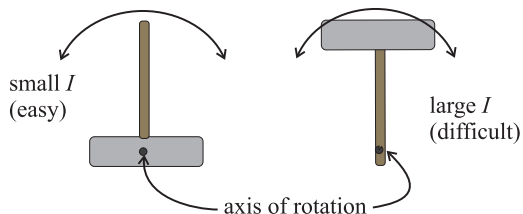
$$I = \sum m_i r_i^2$$

the rotational kinetic energy can be written

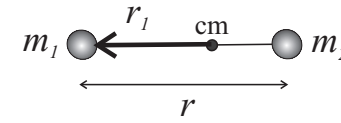
$$K_{\text{ang}} = \frac{1}{2}I\omega^2 \quad (\text{cf. } K_{\text{lin}} = \frac{1}{2}mv^2)$$

The moment of inertia plays a similar role in rotational motion as mass does in linear motion.

The magnitude of I depends on the axis of rotation.



Classical rotation of diatomic molecules

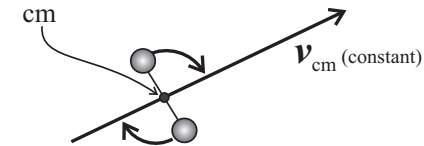


For a diatomic molecule with a bondlength r , rotation must occur about the CM¹⁰, and the moment of inertia can be written (using $\sum_i m_i r_i = 0$)

$$I = \sum_i m_i r_i^2 = \mu r^2 \quad \text{with } \mu = \frac{m_1 m_2}{m_1 + m_2}$$

In the absence of external forces on the molecule, the motion of the CM is conserved, and the total kinetic energy of the molecule can be factored

$$K = K_{\text{CM}} + K_{\text{ang}}$$

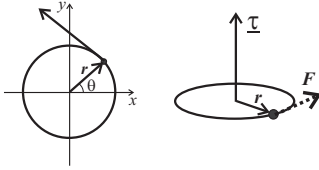


Because both atoms rotate with the same frequency ω about the CM, the angular momentum and the angular kinetic energy of the molecule may be written (see below)

$$l = \sum_i m_i r_i^2 \omega = I\omega \quad K_{\text{ang}} = \frac{1}{2} \sum_i m_i r_i^2 \omega^2 = \frac{l^2}{2I}$$

¹⁰Otherwise the motion of the centre-of-mass would not be uniform in the absence of external forces.

Torque and Angular momentum



Consider the work done by force, \mathbf{F} , on an object at fixed distance r from the axis of rotation

$$dW = F_x dx + F_y dy$$

or in angular coordinates (using $dy = x d\theta$ and $dx = -y d\theta$)

$$dW = (xF_y - yF_x) d\theta$$

This can be written

$$dW = \tau d\theta \quad (\text{cf. } dW = F_x dx)$$

where the *torque* is defined

$$\tau = (xF_y - yF_x) = \mathbf{r} \times \mathbf{F}$$

Is it possible to define the torque in terms of a derivative of a momentum, cf. $\mathbf{F} = d\mathbf{p}/dt$?

Try defining the *angular momentum*

$$\mathbf{L} = \mathbf{r} \times \mathbf{p}$$

Then taking the time derivative we obtain

$$\frac{d\mathbf{L}}{dt} = \mathbf{r} \times \mathbf{F} = \tau$$

i.e.

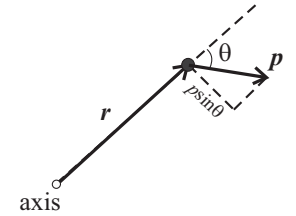
$$\tau = \frac{d\mathbf{L}}{dt} \quad (\text{cf. } \mathbf{F} = d\mathbf{p}/dt)$$

Angular Momentum

For a particle with linear momentum \mathbf{p} , located at position \mathbf{r} , the magnitude of the angular momentum is defined

$$l = rp \sin \theta$$

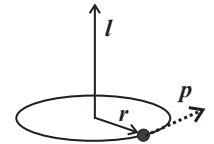
where θ is the angle between \mathbf{r} and \mathbf{p} .



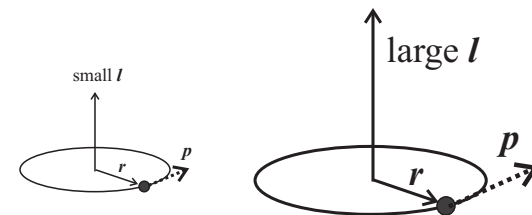
Angular momentum is a vector quantity

It is directed perpendicular to the plane of rotation (as defined by the right hand rule). In vector notation

$$\mathbf{l} = rp \sin \theta \hat{\mathbf{n}} \equiv \mathbf{r} \times \mathbf{p}$$

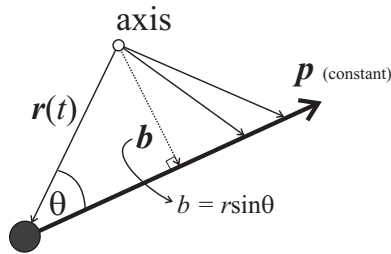


where the latter equation defines the *vector product* between the vectors \mathbf{r} and \mathbf{p} . $\hat{\mathbf{n}}$ is a vector of unit length pointing at right angles (normal) to the plane of rotation.



1. Linear motion

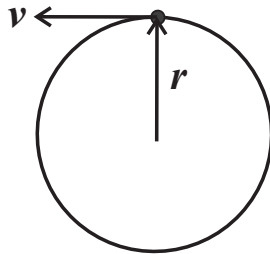
For *motion in straight line*, the angular momentum about any point is constant.



$$l = p r \sin \theta = p b = m v b = \text{constant}$$

2. Uniform motion in a circle

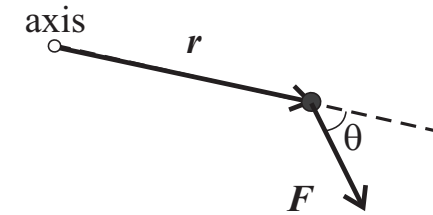
For *uniform motion in a circle* (i.e. no angular acceleration) \mathbf{p} and \mathbf{v} are constant in magnitude and always directed perpendicular to \mathbf{r} , and the angular momentum has a constant magnitude



$$l = mvr = mr^2\omega = I\omega$$

(cf. $p = mv$)

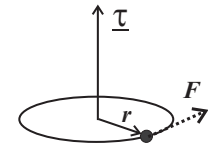
Torque and angular momentum conservation



$$\mathbf{l} = r p \sin \theta \hat{\mathbf{n}} = I\omega$$

The time derivative of the angular momentum defines the torque exerted on the system

$$\boldsymbol{\tau} = \frac{d\mathbf{l}}{dt} = r F \sin \theta \hat{\mathbf{n}} = I\alpha$$



This the rotational analogue of the linear equation

$$\mathbf{F} = \frac{d\mathbf{p}}{dt} = m\mathbf{a}$$

If there is no external torque acting on a system, the total angular momentum is constant in magnitude and direction.

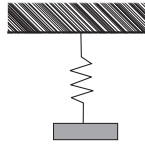
SEE EXAMPLES 8-10

LECTURE 4: Vibrational Motion

Simple Harmonic Motion

Potential Energy:

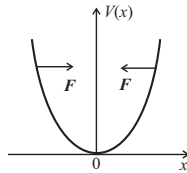
$$V(x) = \frac{1}{2}kx^2$$



where x is the displacement from the rest (or equilibrium) position, and k is known as the *force constant*.

Force:¹¹

$$F(x) = -dV(x)/dx = -kx \equiv -kx(t)$$



The minus sign indicates a *restoring force*.

Acceleration:

$$a = -\frac{k}{m}x(t) = -\omega^2x(t)$$

where

$$\omega = \sqrt{\frac{k}{m}}$$

and is known as the *angular frequency* (for reasons given below).

Thus, the equation of motion for the simple harmonic oscillator is a *second order differential equation*.

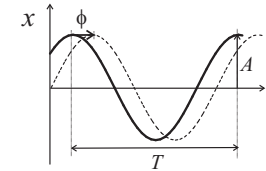
$$\frac{d^2x}{dt^2} = -\omega^2x$$

¹¹When applied to springs, this equation for the force is known as Hooke's law and k is then referred to as the *spring constant*.

We will just quote the solution:

$$x(t) = A \sin(\omega t + \phi)$$

where ϕ determines the *phase* and A defines the *amplitude* of the oscillation.



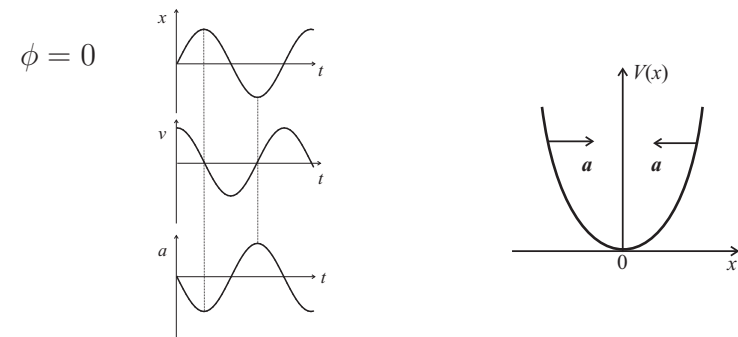
Periodic motion

Taking the time derivative of $x(t)$ yields the velocity $v(t)$

$$v(t) = A\omega \cos(\omega t + \phi)$$

and the second derivative gives the acceleration

$$a(t) = -A\omega^2 \sin(\omega t + \phi) = -\omega^2x(t)$$



As with circular motion, the frequency, f , and period, T , are related to ω by the equations

$$\omega = 2\pi f = \frac{2\pi}{T}$$

An Aside:

Very similar equations arise for uniform circular motion, where the equation of motion is (see Lecture 3):

$$\mathbf{a}_r = \frac{d^2\mathbf{r}}{dt^2} = -\omega^2\mathbf{r} \equiv -r\omega^2\hat{\mathbf{r}}$$

which can be resolved into x and y components

$$a_{r_x} = \frac{d^2r_x}{dt^2} = -\omega^2r_x$$

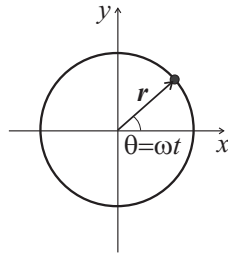
and

$$a_{r_y} = \frac{d^2r_y}{dt^2} = -\omega^2r_y$$

The solution to these equations is

$$r_x = r \cos(\omega t) \equiv r \sin(\omega t + \pi/2)$$

$$r_y = r \sin(\omega t)$$



where the phase $\pi/2$ in the first equation is chosen so that r satisfies the equation for motion confined to a circle

$$r = \sqrt{r_x^2 + r_y^2}$$

Energy in Simple Harmonic Motion

Potential Energy:

$$V(t) = \frac{1}{2}kx^2$$
$$x(t) = A \sin(\omega t + \phi)$$

$$V(t) = \frac{1}{2}kA^2 \sin^2(\omega t + \phi)$$

Kinetic Energy:

$$K(t) = \frac{1}{2}mv^2$$
$$v(t) = A\omega \cos(\omega t + \phi)$$
$$K(t) = \frac{1}{2}mA^2\omega^2 \cos^2(\omega t + \phi)$$

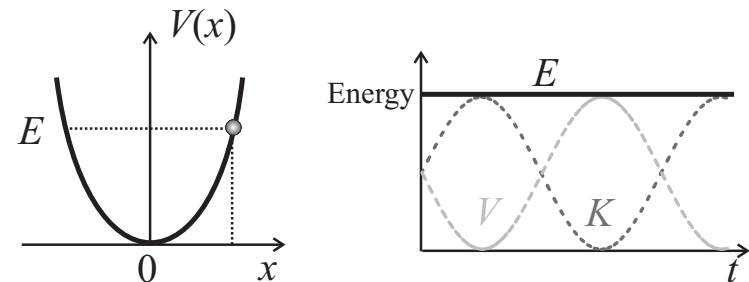
$$K(t) = \frac{1}{2}kA^2 \cos^2(\omega t + \phi)$$

Total Energy:

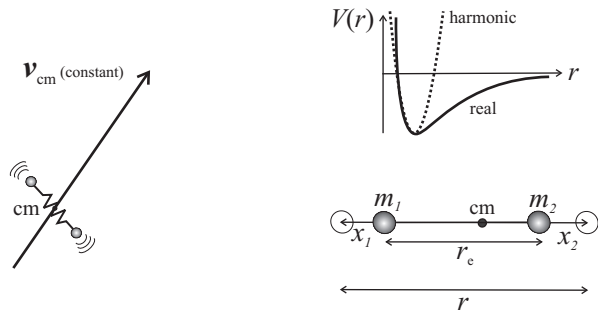
$$E = K + V$$

$$E = \frac{1}{2}kA^2 [\sin^2(\omega t + \phi) + \cos^2(\omega t + \phi)] = \frac{1}{2}kA^2$$

The vibrational frequency of a harmonic oscillator is independent of the total energy.



Vibration of a diatomic molecule



In the absence of external forces the motion of the CM can be factored from the relative motion of the two atoms. The latter is the time dependent bondlength of the molecule:

$$r = r_1 - r_2 = x + r_e \quad \text{where } x = x_1 - x_2$$

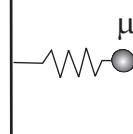
and r_e is the equilibrium bond length of the molecule. Taking the second derivative with respect to time

$$a = a_1 - a_2 = \ddot{x}$$

Using Newton's 3rd Law

$$F_1 = -F_2 = -kx$$

Therefore

$$a = a_1 - a_2 = \left(\frac{-kx}{m_1} - \frac{kx}{m_2} \right) = -\frac{k}{\mu} x = -\omega^2 x$$


where

$$\mu = \frac{m_1 m_2}{(m_1 + m_2)} \quad \text{and} \quad \omega = \sqrt{\frac{k}{\mu}}$$

μ is the *effective mass* of the oscillator and ω is its *angular frequency*.

SEE EXAMPLE 11

Travelling Waves

Travelling harmonic waves possess two periodicities, one in position and one in time:

$$y(x') = A \sin kx' \quad \text{Fixed time}$$

where k (NOT to be confused with the force constant) is known as the *wave number*, i.e. the number of waves per meter in units of rad m^{-1} ,

$$k = \frac{2\pi}{\lambda}$$

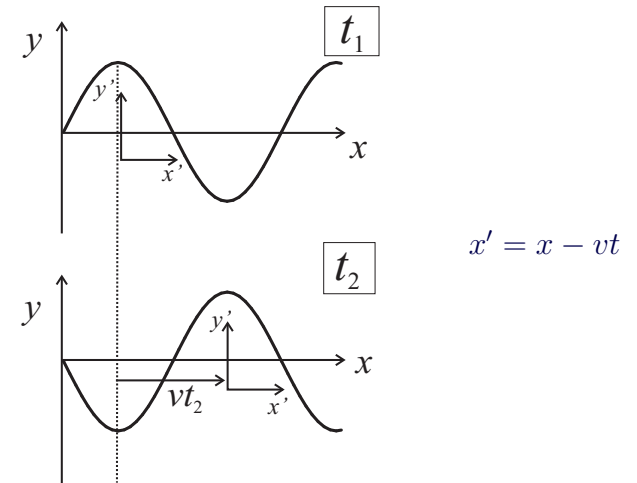
and

$$y(t) = A \sin \omega t \quad \text{Fixed position}$$

with

$$\omega = \frac{2\pi}{T} = 2\pi f$$

as previously.



For a wave travelling with a constant *wave velocity*, v , any particular feature, such as a crest, is defined by a fixed value of x' , where x' refers to the displacement with respect to a coordinate system travelling with the wave. With respect to a stationary frame (the ground) the displacement x , is related to x' by

$$x' = x - vt = \text{constant}$$

Substitution into the first equation yields

$$y(x, t) = A \sin [k(x - vt) + \phi] = A \sin [kx - \omega t + \phi]$$

where the phase, ϕ , is defined at $x = 0$ and $t = 0$, and

$$v = f\lambda$$

such that

$$kv = \frac{2\pi}{\lambda} f\lambda = \omega$$

Linear Wave Equation - an aside

Differentiate the *wave function*

$$y(x, t) = A \sin [k(x - vt) + \phi] = A \sin [kx - \omega t + \phi]$$

with respect to t at fixed x twice (known as *partial differentiation*)

$$\frac{\partial^2 y}{\partial t^2} = -A\omega^2 \sin [kx - \omega t + \phi] = -\omega^2 y(x, t)$$

Repeat the (partial) differentiation of the wave function, but now with respect to x at fixed t :

$$\frac{\partial^2 y}{\partial x^2} = -Ak^2 \sin [kx - \omega t + \phi] = -k^2 y(x, t)$$

Combining these two equations, making use of the definition of the wave velocity, v , yields the linear wave equation

$$\frac{\partial^2 y}{\partial x^2} = \frac{1}{v^2} \frac{\partial^2 y}{\partial t^2}$$

where the partial derivative on the right side of the equation is the acceleration of an element (particle) in the medium.

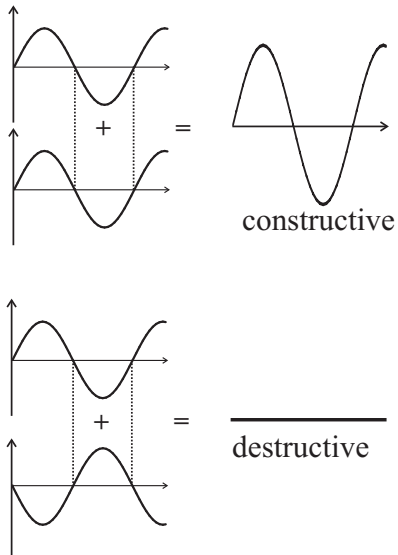
Principle of Linear Superposition

Waves which satisfies the linear wave equation obey the *principle of linear superposition*.

This states that the total wave function, y_{tot} , is the linear sum of the individual wave functions, y_i :

$$y_{\text{tot}} = \sum_i y_i$$

Constructive (destructive) interference occurs when two or more waves add *in (out of) phase* such that the total displacement is greater (less) than the displacements generated by the individual waves.



Interference is an important phenomenon in Quantum Mechanics, and in Optics (e.g., diffraction).

Standing Waves

A *standing wave* may be constructed by superposition of two harmonic waves, of equal amplitude and frequency, travelling in opposite directions.

Setting the phase of each wave to zero, yields the superposition wave

$$y(x, t) = A \sin(kx - \omega t) + A \sin(kx + \omega t)$$

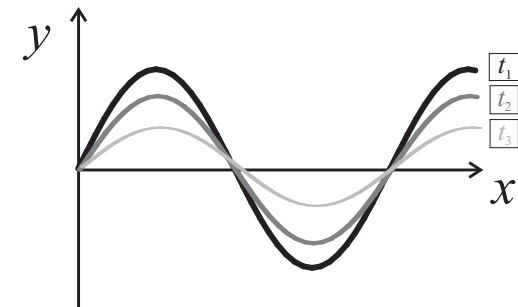
which, using the identity

$$\sin A + \sin B = 2 \sin [(A + B)/2] \cos [(A - B)/2]$$

reduces to

$$y(x, t) = 2A \cos(\omega t) \sin(kx) \equiv A(t) \sin(kx)$$

The latter equation shows that for a standing wave the amplitude varies with time, but the phase of the oscillation along x is invariant with time.



Resonant standing waves

These are produced when the standing wave is fixed at two points in space, such as $x = 0$ and $x = l$.

An example is the wave motion generated in a stringed instrument.

The constraint imposes ***boundary conditions*** to the wave motion

$$y(x = 0, t) = A(t) \sin(k \cdot 0) = 0$$

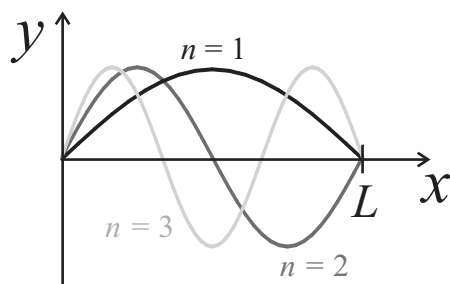
$$y(l, t) = A(t) \sin(kl) = 0$$

This can be fulfilled either by setting the amplitude $A(t) = 0$ (which means the wave no longer exists), or by the constraint $\sin(kl) = 0$, i.e.

$$kl = n\pi \quad n = 1, 2, 3, \dots \text{ etc.}$$

or

$$\lambda = \frac{2l}{n} \quad (\text{harmonics})$$



cf., matter waves

The behaviour is analogous to that of a quantum mechanical particle confined to a box (see Physical Chemistry Lectures).

SEE EXAMPLE 12