

PRINCIPLES OF PHYSICAL CHEMISTRY: CLASSICAL MECHANICS

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LECTURE OUTLINE

1. NEWTON'S LAWS OF MOTION.
2. MOMENTUM, WORK AND ENERGY.
3. ROTATIONS: ANGULAR MOMENTUM AND MOMENTS OF INERTIA.
4. VIBRATIONS: SIMPLE HARMONIC MOTION.

RECOMMENDED TEXTBOOKS

FOUNDATIONS OF PHYSICS FOR CHEMISTS.

Ritchie & Sivia. Oxford Chemistry Primer covering most of the material in this course. I expect you to read this book.

ELEMENTS OF PHYSICAL CHEMISTRY.

Atkins & de Paula. Chapter 1 covers some of the material in this course.

PHYSICS.

Alonso & Finn. Physics textbook covering this course and much more besides.

UNIVERSITY PHYSICS.

Benson. Another alternative University physics textbook.

ONLINE MATERIAL

Handouts, slides, and problem sets can be found at www.markwallace.org

EQUATIONS OF MOTION IN ONE DIMENSION

The motion, or trajectory, of a particle is defined by its position, velocity, and acceleration.

Position	m	$r_x(t)$
Velocity	ms^{-1}	$v_x(t) = \frac{dr_x}{dt} \equiv \dot{r}_x$
Acceleration	ms^{-2}	$a_x(t) = \frac{dv_x}{dt} = \frac{d^2r_x}{dt^2} \equiv \ddot{r}_x$

AN EXAMPLE: CALCULATING ACCELERATION

We can calculate the acceleration of a particle given its time dependent position. Let us choose an arbitrary function describing particle position:

$$r_x(t) = At^3$$

$$v_x(t) = \frac{dr_x}{dt} = 3At^2$$

$$a_x(t) = \frac{dv_x}{dt} = 6At$$

AN EXAMPLE: CALCULATING POSITION

Similarly, we can calculate the position of a particle given its time dependent acceleration:

$$a_x(t) = 6At$$

$v_x(t)$ is obtained by integration

$$v_x(t) = \int a_x(t) dt = \int 6At dt = 3At^2 + C$$

Let us set $r=0$ and $v=0$ at $t=0$. Integrating again gets us back to the position:

$$r_x(t) = \int v_x(t) dt = \int 3At^2 dt = At^3$$

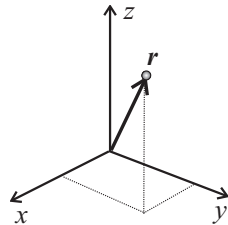
EQUATIONS OF MOTION FOR CONSTANT ACCELERATION

Use the above treatment to show that for constant acceleration, $a_x(t) = a$ a particle's position is described by

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

EQUATIONS OF MOTION IN THREE DIMENSIONS

Obviously we must be able to describe particles that move in more than one dimension



For constant acceleration

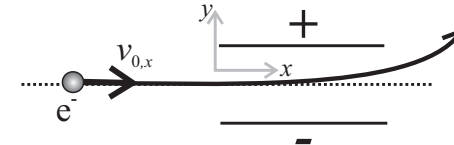
$a_x(t) = a_x$	$v_x(t) = v_{x0} + a_x t$	$r_x(t) = r_{x0} + v_{x0}t + \frac{1}{2}a_x t^2$
$a_y(t) = a_y$	$v_y(t) = v_{y0} + a_y t$	$r_y(t) = r_{y0} + v_{y0}t + \frac{1}{2}a_y t^2$
$a_z(t) = a_z$	$v_z(t) = v_{z0} + a_z t$	$r_z(t) = r_{z0} + v_{z0}t + \frac{1}{2}a_z t^2$

Motion in each orthogonal direction can be decomposed into a separate set of equations. This is often a useful tool for breaking down a problem into more manageable parts. We can also combine these equations by describing the motion with vectors.

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

AN EXAMPLE: THE CATHODE RAY TUBE

Electrons, initially travelling at $2.4 \times 10^6 \text{ m s}^{-1}$ in the horizontal direction, enter a region between two horizontal charged plates of length 2 cm where they experience an acceleration of $4 \times 10^{14} \text{ m s}^{-2}$ vertically upwards. Find (a) the vertical position as they leave the region between the plates, and (b) the angle at which they emerge from between the plates.



For motion along the x coordinate,

$$\begin{aligned} a_x &= 0 \\ v_x &= v_{0x} = 2.4 \times 10^6 \text{ m s}^{-1} \\ r_x &= r_{0x} + v_{0x}t \quad (r_{0x} = 0) \\ r_x &= 2.4 \times 10^6 t = 0.02 \text{ m} \\ \therefore t &= 8.33 \times 10^{-9} \text{ s} \end{aligned}$$

For motion along the y coordinate,

$$\begin{aligned} a_y &= 4 \times 10^{14} \text{ m s}^{-2} \\ v_y &= v_{0y} + a_y t \quad (v_{0y} = 0) \\ r_y &= r_{0y} + \frac{1}{2}a_y t^2 \quad (r_{0y} = 0) \end{aligned}$$

Substitute for the time the electron spends between the plates,

$$r_y = \frac{1}{2}a_y t^2 = 0.0139 \text{ m}$$

For the angle at which the electrons depart,

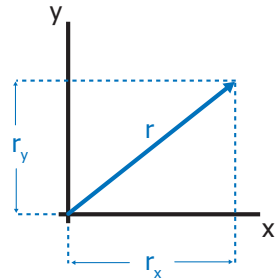
$$\tan \theta = \frac{v_y}{v_x} = \frac{a_y t}{v_{0x}} \qquad \theta = 54.2^\circ$$

VECTOR REVISION

A vector is a quantity with both magnitude and direction. Vectors will be covered in detail in your mathematics course.

AN EXAMPLE: 2D VECTORS

Consider a position vector r with magnitude r and direction θ with respect to the x axis. We can decompose this vector into two orthogonal components r_x and r_y .



COMPONENTS

$$r_x = |r| \cos \theta \quad r_y = |r| \sin \theta$$

MAGNITUDE

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

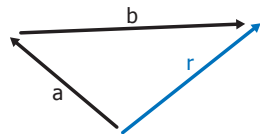
DIRECTION

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

The vector r can be described as the sum of its two components, r_x and r_y , each multiplied by their respective unit vectors i and j . Unit vectors are vectors with a magnitude of 1 in their respective direction.

$$\vec{r} = r_x \vec{i} + r_y \vec{j}$$

VECTOR ADDITION



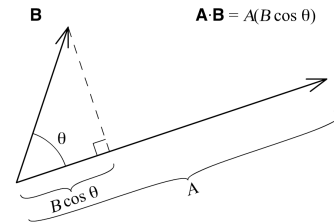
$$\vec{r} = \vec{a} + \vec{b}$$

$$r_x = a_x + b_x \quad r_y = a_y + b_y$$

VECTOR MULTIPLICATION

When two vectors are multiplied we must deal with not only the magnitude, but also the direction of the resultant vector. Multiplication of one vector by another is not uniquely defined. Consider two vectors A and B .

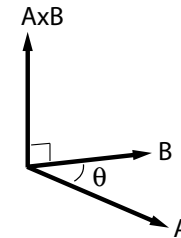
SCALAR (DOT) PRODUCT



$$\vec{A} \cdot \vec{B} = |A||B| \cos \theta$$

The dot product is a scalar quantity.

VECTOR (CROSS) PRODUCT



$$\vec{A} \times \vec{B} = \hat{n}|A||B| \sin \theta$$

The cross product is a vector quantity.
 \hat{n} is a unit vector perpendicular to the plane containing A and B .

NEWTON'S LAWS OF MOTION

N1: AN OBJECT IN MOTION WILL REMAIN IN MOTION UNLESS ACTED UPON BY A NET FORCE.

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

N2: $F = ma$. A FORCE ACTING ON A BODY IS DIRECTLY PROPORTIONAL TO ITS RATE OF CHANGE OF MOMENTUM.

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

N3: TO EVERY ACTION THERE IS AN EQUAL AND OPPOSITE REACTION.

Tells us about how forces operate.

ARE THE LAWS ALWAYS CORRECT?

No! But they are often a very good approximation.

WHAT DO THE LAWS TELL US?

They enable us to predict the motion of particles. To understand them fully, we're going to first require a few more physical concepts:

FORCES

A force is any influence which tends to change the motion of an object. Forces are inherently vector quantities.

TYPES OF FORCE

Fundamental Force	Relative Strength	Range	Comments
Strong	1	10^{-15} m	Holds the nucleus together.
Electromagnetic	10^{-2}	∞	Chemistry!
Weak	10^{-6}	10^{-17} m	Associated with radioactivity.
Gravitational	10^{-38}	∞	Causes apples to fall.

For most problems in chemistry, we only need worry about electromagnetic forces.

GRAVITATIONAL FORCES

The gravitational force between point or spherical masses, m_1 and m_2 , is

$$F = -\frac{Gm_1m_2}{r^2}$$

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

The weight of an object is the net gravitational force acting on it. For objects close to the earth's surface ($r = R_e$):

$$F = mg$$

$$g = \frac{Gm_E}{R_e^2} \simeq 9.8 \text{ m s}^{-2}$$

where g is the acceleration due to gravity.

ELECTROSTATIC FORCES

In a vacuum, the Coulomb force between point or spherical charges, q_1 and q_2 , is

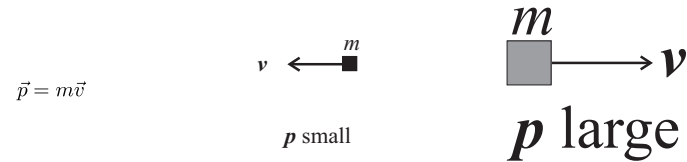
$$F = \frac{q_1q_2}{4\pi\epsilon_0r^2}$$

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

Unlike gravity (which is always attractive), the Coulomb force can be either attractive or repulsive depending on the sign of the charges. Electrostatics will be covered in detail in the Electricity and Magnetism course.

CONSERVATION OF MOMENTUM. THE TOTAL MOMENTUM OF AN ISOLATED SYSTEM OF PARTICLES IS CONSTANT.

Momentum, p is the product of an objects mass times its velocity.

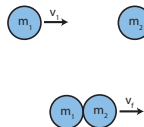


Newton's laws embed the idea of conservation of linear momentum. In a closed system, momentum is always conserved. The principle of conservation of momentum can be stated in it's most general form as:

$$\vec{P} = \sum_i \vec{p}_i = \vec{p}_1 + \vec{p}_2 + \vec{p}_3 + \dots = \text{constant}$$

AN EXAMPLE: INELASTIC COLLISIONS

A particle of mass m travelling at a velocity v hits a stationary particle of the same mass and sticks to it. What is the final velocity v_f of the two particles after they collide?



In an inelastic collision, momentum is conserved, but kinetic energy is not.

Momentum before collision?

$$\sum_i p_i = m_1 v_1 + m_2 v_2 = mv + 0 = mv$$

Momentum after collision?

$$\sum_i p_i = (m_1 + m_2) v_f = 2mv_f$$

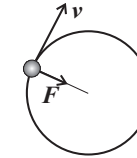
Applying conservation of momentum

$$mv = 2mv_f$$

Hence $v_f = v/2$.

NEWTON'S 1ST LAW. AN OBJECT IN MOTION WILL REMAIN IN MOTION UNLESS ACTED UPON BY A NET FORCE.

This implies that changes in velocity (i.e. acceleration) arise from forces.



NEWTON'S 2ND LAW. $F=MA$. A FORCE ACTING ON A BODY IS DIRECTLY PROPORTIONAL TO ITS RATE OF CHANGE OF MOMENTUM.

Newton's second law describes the observation that the acceleration of an object depends directly upon the net force acting upon the object, and inversely upon the mass of the object.

Newton's Second Law can be expressed in terms of the linear momentum:

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

We can rewrite this equation in a more familiar form knowing that momentum, $p=mv$ and for cases where the mass of our object does not change

$$\vec{F} = \frac{d\vec{p}}{dt} = \frac{d(m\vec{v})}{dt} = m \frac{d\vec{v}}{dt} = m\vec{a}$$

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

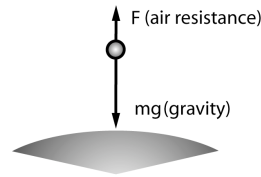
Force has units of Newtons (1 N = 1 kg m s⁻²). Force is a vector quantity, and can therefore be decomposed into orthogonal components. If more than one force acts on a particle, the net force determines the acceleration of the particle

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

AN EXAMPLE: SKYDIVING!

If we know the force acting on an object, we can calculate the particle's motion.

$$m\ddot{a} = \sum_i \vec{F}_i = mg - F_{air}$$



Assuming in this example that the retarding force due to air resistance can be described by $F_{air} = kv$, where k is a constant, and v is the velocity. We can calculate the terminal velocity of the object.

$$a = \frac{dv}{dt} = \frac{mg}{m} - \frac{kv}{m}$$

This differential equation can be solved by separating the variables v and t , and integrating:

$$\int \frac{dv}{g - \frac{k}{m}v} = \int dt + C$$

$$-\frac{m}{k} \ln\left(g - \frac{k}{m}v\right) = t + C$$

Setting $v=0$ when $t=0$

$$v = \frac{mg}{k} (1 - e^{-\frac{k}{m}t})$$

as $t \rightarrow \infty$, $v \rightarrow v_T$ so $v_T = mg/k$.

AN EXAMPLE: THE HYDROGEN ATOM

The force of attraction between the electron and the proton in a hydrogen atom is $F = 8.2 \times 10^{-8}$ N. The mass of the electron is 9.109×10^{-31} kg and that of the proton is 1.672×10^{-27} kg. Calculate the acceleration of each particle due to their mutual interaction.

NEWTON'S 3RD LAW. TO EVERY ACTION THERE IS AN EQUAL AND OPPOSITE REACTION.

$$F_{AB} = -F_{BA}$$

Newton's third law describes the phenomenon that if a force is exerted by one object on another, there is an equal and opposite force acting on the first object.

AN EXAMPLE: MORE SKYDIVING!

Ignoring air resistance, calculate the change in position of the earth just before impact when an unlucky skydiver falls from a position 1 km above the surface of the earth.

Using NIII and NII:

$$\begin{aligned} F_{AE} &= -F_{EA} \\ m_A a_A &= -m_E a_E \\ a_E &= g \frac{m_A}{m_E} \\ a_E &= 1.07 \times 10^{-22} \text{ ms}^{-2} \end{aligned}$$



So how long until the skydiver hits?

$$\begin{aligned} r &= r_0 + v_0 t + \frac{1}{2} a t^2 \\ 0 &= 1000 + 0 - \frac{1}{2} g t^2 \\ t &= 14.3 \text{ s} \end{aligned}$$

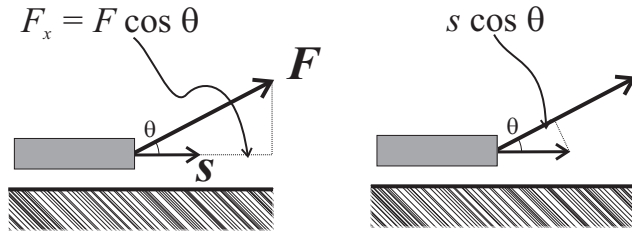
How far did the earth move in that time?

$$\begin{aligned} r &= r_0 + v_0 t + \frac{1}{2} a t^2 \\ r &= 0 + 0 + \frac{1}{2} a_E t^2 \\ r &= 10^{-20} \text{ m} \end{aligned}$$

Unsurprisingly, that's not very far!

WORK

The concept of mechanical work provides the link between force and energy. Work is done on an object when a force acts on it in the direction of motion.



The mechanical work, W , done by a constant force, F , is simply the force times the total displacement, s , in the direction of the force. This is most easily described vector notation as a scalar product;

$$W = \vec{F} \cdot \vec{s}$$

In the example above, the work done will be

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

Notice that the work done is a scalar quantity. If the displacement in the direction of the force is zero, no work is done. If the work when the force is not constant we need to extend our definition. The work done in by a force acting on an object in a constant direction is

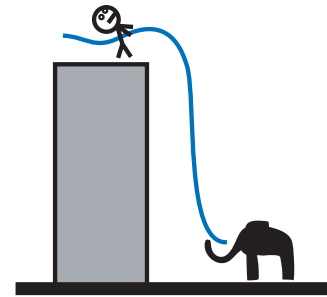
$$W = \int_{x_1}^{x_2} F_x dx$$

where dx is the infinitesimal displacement along x . If the movement is not in a constant direction, again we need to extend our mathematical description a little further.

$$W = \int_C \vec{F} \cdot d\vec{s}$$

Here C describes the path taken during the motion. We also need to include the scalar product here to cope with the fact that we must treat both force and displacement as vectors.

AN EXAMPLE: LIFTING ELEPHANTS



Your lecturer decides to haul an Asian Bull Elephant to the roof of the Chemistry Research Laboratory, using a steel cable weighing 500 g per metre. Assuming the CRL is 100 m high, and that the average weight of an Asian Bull Elephant is 2300 kg, calculate the work done.

Dealing with the elephant first:

$$W = F s = (mg)s = 2300 \times 9.8 \times 100 = 2.25 \times 10^6 \text{ J}$$

Now the cable:

$$W = \int_0^{100} F ds = \int_0^{100} (mg)s ds = 0.5 \times 9.8 \left[\frac{s^2}{2} \right]_0^{100} = 2.45 \times 10^4 \text{ J}$$

So in total:

$$W = 2.28 \times 10^6 \text{ J}$$

KINETIC ENERGY

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

$$K = \frac{1}{2}mv_x^2$$

Returning to the equation for the work done on a particle

$$W = \int F_x dx$$

Use Newton's 2nd Law to rewrite

$$F_x dx = ma_x dx = m \frac{dv_x}{dt} dx = mv_x dv_x$$

gives

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

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

$$W = \Delta K$$

AN EXAMPLE: THE CATHODE RAY TUBE REVISITED

An electron accelerated in a TV tube reaches the screen with a kinetic energy of 10 000 eV. Find the velocity of the electron.

We must first convert from eV into Joules.

$$K = 10^4 \text{ eV} = 10^4 \times 1.6 \times 10^{-19} \text{ J} = 1.6 \times 10^{-15} \text{ J}$$

Before calculating the velocity

$$v = \sqrt{\frac{2K}{m}} = \sqrt{\frac{2 \times 1.6 \times 10^{-15}}{9.109 \times 10^{-31}}} = 5.93 \times 10^7 \text{ ms}^{-1}$$

Pretty fast!

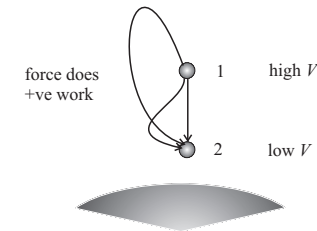
POTENTIAL ENERGY

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.

THE LINK BETWEEN FORCE, WORK AND POTENTIAL ENERGY.

For some forces the work done by the force is independent of the path taken. Such forces are called conservative forces and include gravity and electrostatic forces. 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.

Consider gravity as an example of a conservative force:



The work done dW by the gravitational force F is independent of the path. 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:

$$dV = -dW$$

As we already know that $W = \int F_x dx$, we can combine these equations to yield

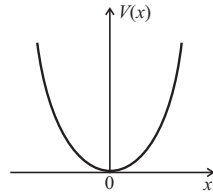
$$F = -\frac{dV}{dx} \quad V(x_2) - V(x_1) = \Delta V = -\int_1^2 F_x dx = -W$$

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

AN EXAMPLE: THE HARMONIC SPRING POTENTIAL

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

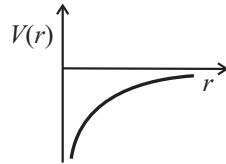
$$F(x) = -\frac{dV}{dx} = -kx$$



AN EXAMPLE: GRAVITATIONAL POTENTIAL

$$V(r) = -\frac{Gm_1m_2}{r}$$

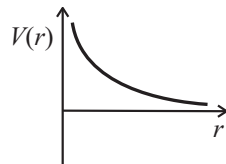
$$F(r) = -\frac{dV}{dr} = -\frac{Gm_1m_2}{r^2}$$



AN EXAMPLE: ELECTROSTATIC POTENTIAL

$$V(r) = \frac{q_1q_2}{4\pi\epsilon_0r}$$

$$F(r) = -\frac{dV}{dr} = \frac{q_1q_2}{4\pi\epsilon_0r^2}$$



(Assuming q_1 and q_2 have the same sign)

CONSERVATION OF ENERGY. THE TOTAL ENERGY IN A CLOSED SYSTEM OF PARTICLES IS CONSTANT.

As shown above, the work done by a force is related to changes in both the kinetic and the potential energies. Again we focus exclusively on conservative forces.

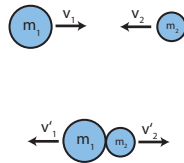
$$W = \Delta K = -\Delta V$$

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:

$$E = K + V$$

ELASTIC COLLISIONS BETWEEN ATOMS

Consider the head-on collision between two atoms. Derive an expression for the final velocity of both particles in terms of their masses and initial velocities assuming the collision is elastic.



In an elastic collision, kinetic energy is conserved, along with total energy and momentum which are always conserved. Collisions in an ideal gas can be considered as perfectly elastic. A perfectly elastic collision implies that there is no change in internal structure of the system, therefore there is no change in potential energy, and hence kinetic energy is conserved. The total energy is conserved during the collision

$$E = K_1 + V_1 + K_2 + V_2 = K'_1 + V'_1 + K'_2 + V'_2$$

As

$$V_1 = V'_1 \quad V_2 = V'_2$$

We can thus show that kinetic energy is indeed conserved.

AN EXAMPLE: ELASTIC COLLISIONS BETWEEN ATOMS

Initial momentum of system:

$$p_i = m_1 v_{i1} + m_2 v_{i2}$$

Final momentum of the system:

$$p_f = m_1 v_{f1} + m_2 v_{f2}$$

Initial kinetic energy of system:

$$K_i = \frac{1}{2} m_1 v_{i1}^2 + \frac{1}{2} m_2 v_{i2}^2$$

Final kinetic energy of the system:

$$K_f = \frac{1}{2} m_1 v_{f1}^2 + \frac{1}{2} m_2 v_{f2}^2$$

Let's apply conservation of momentum,

$$\begin{aligned} m_1 v_{i1} + m_2 v_{i2} &= m_1 v_{f1} + m_2 v_{f2} \\ m_1 (v_{i1} - v_{f1}) &= m_2 (v_{i2} - v_{f2}) \end{aligned} \quad \text{---1}$$

and similarly, conservation of kinetic energy as it is an elastic collision.

$$\begin{aligned} m_1 v_{i1}^2 + m_2 v_{i2}^2 &= m_1 v_{f1}^2 + m_2 v_{f2}^2 \\ m_1 (v_{i1}^2 - v_{f1}^2) &= m_2 (v_{i2}^2 - v_{f2}^2) \end{aligned} \quad \text{---2}$$

We can solve these two simultaneous equations to determine the final velocities, but it may not be immediately obvious how to do it. One route is to note that $a^2 - b^2 = (a+b)(a-b)$ and substitute into 2.

$$m_1 (v_{i1} + v_{f1})(v_{i1} - v_{f1}) = m_2 (v_{i2} + v_{f2})(v_{i2} - v_{f2}) \quad \text{---3}$$

3 / 1 then gives us

$$v_{i1} + v_{f1} = v_{i2} + v_{f2} \quad \text{---4}$$

You could express this in words as the difference in initial velocities is equal to the difference in final velocities. We can the sub this expression into 1 or 2 to retrieve the final velocities in terms of the initial conditions:

Take 4 and multiply by m_1

$$m_1 v_{i1} + m_1 v_{f1} = m_1 v_{i2} + m_1 v_{f2}$$

Add this to 1 giving

$$\begin{aligned} m_1 v_{i1} + m_2 v_{i2} + m_1 v_{i1} - m_2 v_{i2} &= m_1 v_{f1} + m_2 v_{f2} + m_1 v_{f2} - m_1 v_{f1} \\ 2m_1 v_{i1} + (m_2 - m_1) v_{i2} &= (m_2 + m_1) v_{f2} \end{aligned}$$

So our expression for the final velocity of particle 2 is

$$v_{f2} = \frac{2m_1}{m_1 + m_2} v_{i1} + \frac{m_2 - m_1}{m_1 + m_2} v_{i2}$$

You can get a similar expression for particle 1.

FRAMES OF REFERENCE

In applying conservation of momentum in the above example, we had to pick a frame of reference. We measured the velocity of m_1 and m_2 relative to a fixed frame of reference. We can link velocity of an object in one frame of reference (v) with motion in another (v') by simply subtracting the relative velocity between the two frames (v_{rel}).

$$\vec{v}' = \vec{v} - \vec{v}_{rel}$$

Conservation of momentum can only be applied within one frame of reference. This concept is often useful for simplifying collisions; in particular in the centre of mass frame of reference the total momentum is zero.

CENTRE OF MASS

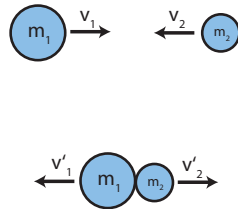
The centre of mass of a system is the point where the system responds as if it were a point with a mass equal to the sum of the masses of its constituent parts. In one-dimension for N particles in a system this is described by

$$Mx_{CM} = \sum_{i=1}^N m_i x_i \qquad M = \sum_{i=1}^N m_i$$

where x_{CM} is the distance to the centre of mass, m_i is a particles mass and x_i is its position. For two particles (such as in a diatomic molecule) this simplifies to

$$(m_1 + m_2) x_{CM} = m_1 x_1 + m_2 x_2$$

AN EXAMPLE: COM FRAME IN COLLISIONS



Take the previous example of an elastic collision between two particles, we could've simplified our calculation by working in the centre of mass frame. In the centre of mass frame, the velocity of the frame is zero, as is the total momentum. Let's denote the velocities in the new frame as v'

Initial momentum of system:

$$0 = m_1 v'_{i1} + m_2 v'_{i2}$$

Final momentum of the system:

$$0 = m_1 v'_{f1} + m_2 v'_{f2}$$

Initial kinetic energy of system:

$$K_i = \frac{1}{2} m_1 v'_{i1}{}^2 + \frac{1}{2} m_2 v'_{i2}{}^2$$

Final kinetic energy of the system:

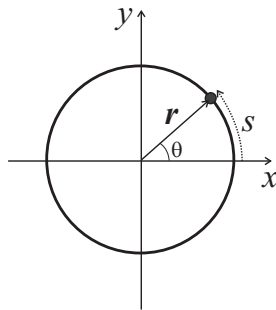
$$K_f = \frac{1}{2} m_1 v'_{f1}{}^2 + \frac{1}{2} m_2 v'_{f2}{}^2$$

Now it's much more straightforward to show

$$\begin{aligned} m_1 v'_{i1}{}^2 + m_2 v'_{i2}{}^2 &= m_1 v'_{f1}{}^2 + m_2 v'_{f2}{}^2 \\ m_1 v'_{i1}{}^2 + m_2 \left(-\frac{m_1}{m_2} v_{i1}\right)^2 &= m_1 v'_{f1}{}^2 + m_2 \left(-\frac{m_1}{m_2} v_{f1}\right)^2 \\ v'_{i1}{}^2 \left(m_1 + \frac{m_1^2}{m_2}\right) &= v'_{f1}{}^2 \left(m_1 + \frac{m_1^2}{m_2}\right) \\ v'_{i1}{}^2 &= v'_{f1}{}^2 \end{aligned}$$

This equation has two solutions. Either $v'_{i1}=v'_{f1}$ which is pretty boring; nothing's happened. Or $v'_{i1}=-v'_{f1}$ (and $v'_{i2}=-v'_{f2}$) which tells us that after the collision the particles have reversed their velocities.

CIRCULAR MOTION



The radian, θ is defined by the equation,

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

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

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

Similarly, we can also have an angular acceleration, α

$$\alpha = \frac{d\omega}{dt} \quad \left(\text{cf. } a = \frac{dv}{dt} \right)$$

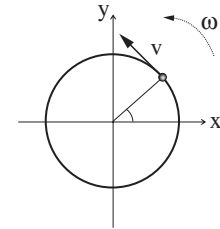
For uniform circular motion, we can define a rotational period, T , and rotational frequency, f related to ω by the equations

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

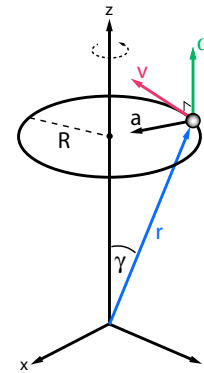
VECTORS IN CIRCULAR MOTION

For a fixed angular velocity, the velocity of a rotating particle, v , must be directly proportional to the radius of rotation, R .

$$v = \omega R$$



Both angular velocity and the particle position are vectors. The angular velocity vector has a direction perpendicular to the plane of motion. Now let's consider vectors from a point of reference that is not simply the centre of rotation



$$\vec{v} = \vec{\omega} \times \vec{r}$$

The magnitude of the velocity, $|v|$, is therefore

$$|v| = |\omega||r| \sin \gamma$$

For uniform circular motion (constant ω) the centripetal acceleration is

$$\vec{a} = \frac{d\vec{v}}{dt} = \vec{\omega} \times \frac{d\vec{r}}{dt}$$

or

$$\vec{a} = \vec{\omega} \times \vec{v}$$

i.e. the centripetal acceleration points radially inwards. It is constant in magnitude but not in direction. As ω is perpendicular to v we can write $a = \omega v$. Remembering that $v = \omega R$

$$a = \omega^2 R = \frac{v^2}{R}$$

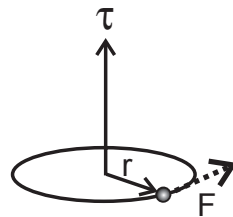
The magnitude of the centripetal force is

$$F = ma = \frac{mv^2}{R}$$

TORQUE AND ANGULAR MOMENTUM

A torque can (very roughly) be considered to be the rotational equivalent of a force. For a force applied perpendicular to r , the torque, τ , is

$$\tau = rF$$



In terms of vector notation

$$\vec{\tau} = \vec{r} \times \vec{F}$$

ANGULAR MOMENTUM. IS IT POSSIBLE TO DEFINE THE TORQUE IN TERMS OF A DERIVATIVE OF A MOMENTUM, LIKE WITH LINEAR FORCES?

Try defining the angular momentum, l

$$\vec{l} = \vec{r} \times \vec{p}$$

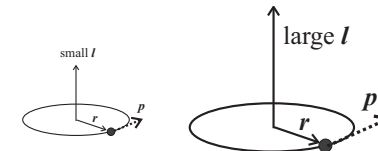
Then taking the time derivative we obtain

$$\frac{d\vec{l}}{dt} = \vec{r} \times \vec{F} = \vec{\tau}$$

i.e.

$$\vec{\tau} = \frac{d\vec{l}}{dt} \quad \left(\text{cf. } \vec{F} = \frac{d\vec{p}}{dt} \right)$$

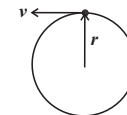
Angular momentum is a vector directed perpendicular to the plane of rotation (as defined by the right hand rule).



ANGULAR MOMENTUM FOR UNIFORM MOTION IN A CIRCLE

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

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



CONSERVATION OF ANGULAR MOMENTUM. IF THERE IS NO EXTERNAL TORQUE ACTING ON A SYSTEM, THE TOTAL ANGULAR MOMENTUM IS CONSTANT IN MAGNITUDE AND DIRECTION.

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 $v = \omega R_i$ where R_i is the particle's distance from the axis of rotation).

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

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

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

Defining the moment of inertia, I , as

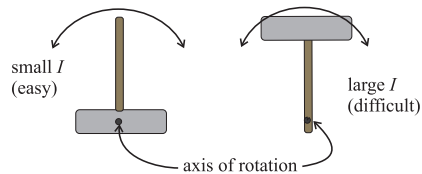
$$I = \sum_i m_i r_i^2$$

the rotational kinetic energy can be written

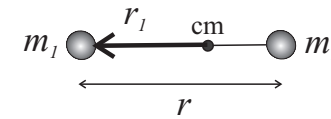
$$K_{\text{ang}} = \frac{1}{2} I \omega^2 \quad (\text{cf. } K_{\text{lin}} = \frac{1}{2} m v^2)$$

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



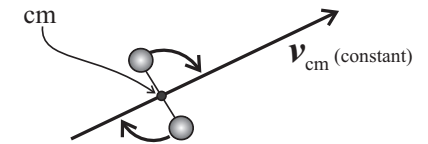
For a diatomic molecule with a bond length r , rotation must occur about the centre-of-mass, and the moment of inertia can be written

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

μ is the reduced mass. Reduced mass is the 'effective' inertial mass. Rather than considering the motion of the molecule, by using the reduced mass we can focus only on the motion of each atom relative to the centre of mass. We can prove this by considering the relative acceleration between the two atoms ($a = a_1 - a_2$) from Newton's third law.

In the absence of external forces on the molecule, the motion of the centre-of-mass 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 as

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

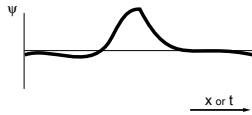
WAVES AND SIMPLE HARMONIC MOTION

THE WAVE EQUATION

In one dimension wave motion can be described by

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

Where ψ is a function that describes the wave (the wave function) and v is the speed of the wave. This equation tells us about how a wave propagates in space and time.



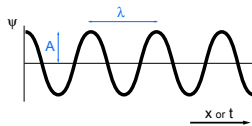
The general solutions to this equation can be expressed as the superposition of two waves propagating in opposite directions.

$$\psi(x, t) = f_1(x - vt) + f_2(x + vt)$$

where f_1 and f_2 are arbitrary functions. The fluctuations in a wave can be perpendicular to the direction of motion (a transverse wave), or parallel to the direction of motion (longitudinal wave).

AN EXAMPLE: SINUSOIDAL WAVES

We can verify that this differential equation really does describe a wave, let's start with the simplest of waves - a sinusoid.



We can draw two equivalent sine waves, describing oscillations in either in position (x) or time (t). The equation for this wave can be written as

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

We can vary either time or position in this equation, and we would see a sinusoidal variation in amplitude of the wave function.

WAVELENGTH, λ , Is the distance between successive peaks.

AMPLITUDE, A , Is the maximum value of the wave function.

FREQUENCY, ν , is the number of cycles per second.

PHASE, ϕ , is the initial offset of the wave in x at time $t=0$.

ANGULAR WAVENUMBER,¹ k , is the number of wavelengths in the distance 2π . $k = 2\pi / \lambda$.

ANGULAR FREQUENCY, ω , is the number of cycles per second, measured in radians. $\omega = 2\pi\nu$.

WAVE VELOCITY², v , Is the speed of the wave. $v = \lambda \nu = \omega / k$.

Don't confuse (angular) wavenumber ($k=2\pi/\lambda$) used when talking about waves, and wavenumber used in spectroscopy. In spectroscopy, wavenumber is the number of wavelengths in one unit of length. It is the spatial analogue of frequency and usually expressed in units of cm^{-1} .

SO IS THIS A SOLUTION TO THE GENERAL WAVE EQUATION?

Differentiate the wave function with respect to t at fixed x twice

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

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

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

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

Combining these two equations, making use of the definition of the wave velocity, $v = \omega / k$, gets

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

us back to the linear wave equation.

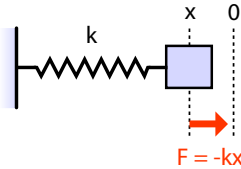
¹ Thus far we have only considered 1D waves, so we don't have to resort to vectors. In this case, \mathbf{k} is called the wave vector and also specifies the direction of propagation of the wave.

² There are several kinds of wave velocity, here we are talking about the group velocity.

SIMPLE HARMONIC MOTION

One easy example of a wave equation is in simple harmonic motion. SHM is present where there is a restoring force that can be considered proportional to the displacement of the system (e.g a pendulum, springs, molecular vibrations, sound waves, etc).

AN EXAMPLE: MASS AND SPRING



Consider the forces on the mass when it is displaced from its resting position by a distance x . We know that $F=ma$. The spring also applies a force given by Hooke's law proportional to the displacement $F_{restoring}=-kx$. Here k is the spring constant.

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

Another second order differential equation! Let's tidy up:

$$\frac{d^2x}{dt^2} + \frac{k}{m}x = 0$$

We can quote a solution:

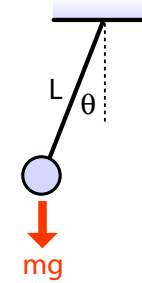
$$x(t) = A \sin(\omega t + \phi)$$

Where $\omega^2=k/m$. ω is again the angular frequency. Check for yourself that this satisfies the differential equation. This gives us.

$$T = \frac{2\pi}{\omega} = 2\pi\sqrt{\frac{m}{k}}$$

Interestingly, the period is independent of the initial displacement. Try and substitute our solution into the differential equation and check it works.

AN EXAMPLE: PENDULUM



The equation of motion for a simple pendulum is given by

$$ma = -mg \sin \theta$$

We can approximate for small angles with

$$\sin \theta \approx \theta$$

So the equation of motion becomes

$$ma = -mg\theta$$

The easiest way to solve this is to convert to an angular form

$$m\alpha L = -mg\theta$$

Giving us the second order differential equation

$$\frac{d^2\theta}{dt^2} + \frac{g}{L}\theta = 0$$

You can use the previous example to show that this can be used to show the period of oscillation is

$$T = 2\pi\sqrt{\frac{L}{g}}$$

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

$$K(t) = \frac{1}{2}mv^2$$

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

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

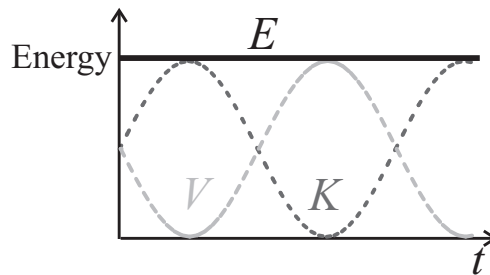
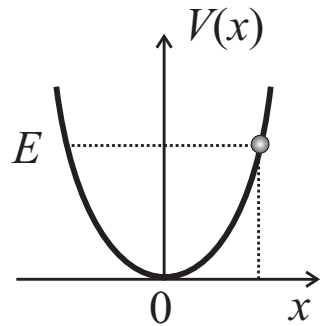
$$K(t) = \frac{1}{2}kA^2 \cos^2(\omega t + \phi)$$

Total energy

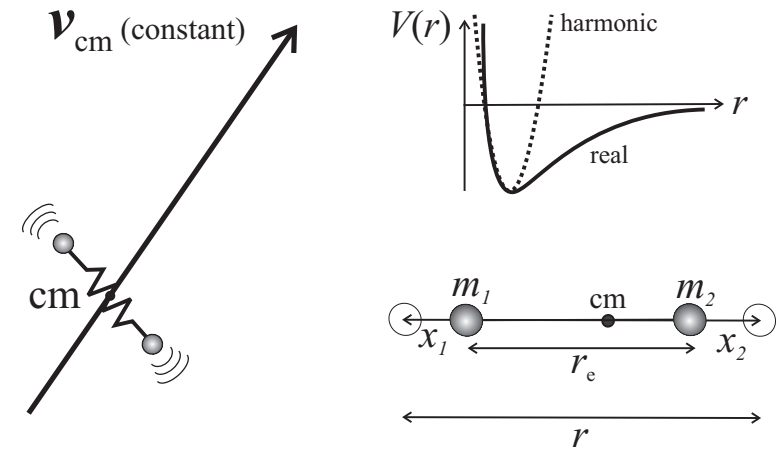
$$E = K + V$$

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

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



VIBRATION OF A DIATOMIC MOLECULE

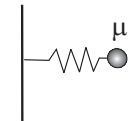


In the absence of external forces, the motion of the CM of a molecule can be treated separately from the relative motion of the two atoms. The relative motion describes the time-dependent changes in bond length of the molecule:

We have an analogous system to a mass on a spring. The only difference here is that we must again use the relative or reduced mass, μ , of the system to only consider the internal motion.

$$\mu = \frac{m_1 m_2}{(m_1 + m_2)}$$

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



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