1ST LECTURE:
MATHEMATICAL FOUNDATIONS AND INTERACTIVE EQUATIONS AND THEIR APPLICATIONS IN QUANTUM CHEMISTRY

الأسس الرياضية والمعادلات التفاعلية وتطبيقاتها في الكيمياء الكمية

الطاقة

Energy:

It is the ability to get a job done

There are types or states of energy, including:

1-kinetic energy   الطاقة الحركيه   K.E   KE   K

2-Potential energy   الطاقة الكامنه (الوضع)   P.E   PE   U

Kinetic energy
الطاقة الحركية

الطاقة يمتلكها الجسم المتحرك

تعتمد على السرعة والكتله

m (kg)   v (m/s)

$$KE = \frac{1}{2} m v^2$$

وحده القياس (جول)

$$kg \cdot \frac{m^2}{s^2} = kg\,m^2/s^2 = J$$

كميه متجهيه

سياره سرعتها 20m/s وكتلتها 10kg ما طاقتها الحركيه

$$KE = \frac{1}{2} m v^2 = \frac{1}{2} (10)(20)^2$$

$$= 2000\,J$$

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potential energy
الطاقة الكامنه (وضع)

الطاقة التي عندك امكانية لكن نتيجة لوضعه (مخزنه)
طاقة الوضع الجاذبيه
الطاقة الكرونيه

$$PE_g = U_g = E_g$$

طاقة الوضع الجاذبيه تعتمد على الكتله والارتفاع

$$E = PE = mgh$$

وحده القياس (جول)

نرفع جسم وزنه على كتله 3kg على بنايه ارتفاعها 10m ما الطاقة المختزنه فيها

$$E = mgh$$
$$= 3(9.8)10$$
$$294\,J$$

1-kinetic energy

طاقة مبتلكها الجيم بسبب الحركة

kinetic energy, form of energy that an object or a particle has by reason of its motion

And from the laws of traditional (classical) mechanics, the kinetic energy of a body of mass ⓜ (Kg) And it moves fast Ⓥ (m/ s) be ½ mv2

كتلة   الحركة

Kinetic Energy

$$K.E. = \frac{1}{2}MV^2$$

M: Mass (Kg)

V: Velocity (m/s)

$$K.E = \frac{1}{2}mv^2$$

كتلة   سرعة

❑ **kinetic energy,** form of energy that an object or a particle has by reason of its motion.

❑ Kinetic energy is a property of a moving object or particle and depends not only on its motion but also on its mass.

❑ The kind of motion may be translation (or motion along a path from one place to another), rotation about an axis, vibration, or any combination of motions.
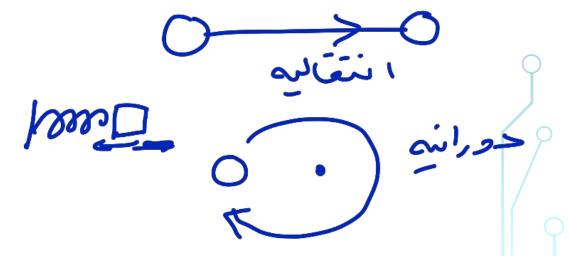
Translational kinetic energy of a body is equal to one-half the product of its mass, m, and the square of its velocity, v, or 1/2mv2.

الطاقة الحركية: هي شكل من أشكال الطاقة التي يمتلكها جسم أو جسيم نتيجةً لحركته.

• الطاقة الحركية خاصية للجسم أو الجسيم المتحرك وتعتمد ليس فقط على حركته، بل أيضًا على كتلته.

• قد تكون الحركة على شكل: انتقال (حركة على مسار من مكان إلى آخر)، أو دوران حول محور، أو اهتزاز، أو مزيج من هذه الحركات.

• الطاقة الحركية الانتقالية لجسم تساوي نصف حاصل ضرب كتلته m في مربع سرعته v، أي:

$$E_k = \frac{1}{2}mv^2$$

E_k = kinetic energy of object
m = mass of object
v = speed of object

The usual SI unit of kinetic energy, is the unit of mass (kg) multiplied by the unit of velocity (m/sec) squared.

$$kg \cdot \left(\frac{m}{sec}\right)^2 = \frac{kgm^2}{sec^2} = J$$

وحدة، لقياس

Notice that this is the same as the unit of work, the Joule. All forms of energy can be measured in Joules.

Examples

كتلة   الحركة

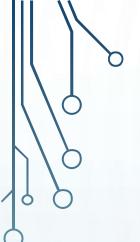1. What is the KE of a White-tailed Jackrabbit of mass 3.4 kg when running at a speed of 15 m/sec?

$$KE = \frac{1}{2}mv^2$$
$$= \frac{1}{2}(3.4\,kg)\left(15\,\frac{m}{sec}\right)^2$$
$$= \frac{1}{2}(3.4\,kg)\,225\,\frac{m^2}{sec^2}$$
$$= 382.5\,\frac{kg\,m^2}{sec^2}$$
$$= 380\,J \quad (rounded)$$

$$KE = \frac{1}{2}mv^2$$
$$= \frac{1}{2}(3.4)(15)^2$$
$$382.5\,J$$

example

mass = 55 kg
velocity = 3.87m/s

$KE = \frac{1}{2}mv^2$

$= \frac{1}{2}(55)(3.87)^2$

$= 411.86 J$

$KE = 0.5 \times mv^2$

$= 0.5 \times 55kg \times (3.87m/s)^2$

$KE = 0.5 \times mv^2$

$= 0.5 \times 55kg \times 14.97m^2/s^2$

$= 411.675 J$

- Example 1: What is the velocity of an object with a mass of 30 kg and a kinetic energy of 500 J?

  v?? *m*

  - $KE = 0.5 \times mv^2$
  - $500\ J = 0.5 \times 30 \times v^2$
  - Multiply mass by 0.5: $0.5 \times 30 = 15$
  - Divide kinetic energy by the product: $500/15 = 33.33$
  - Square root to find velocity: 5.77 m/s

- Example 2: What is the mass of an object with a kinetic energy of 100 J and a velocity of 5 m/s?

  ??

  - $KE = 0.5 \times mv^2$
  - $100\ J = 0.5 \times m \times 5^2$
  - Square the velocity: $5^2 = 25$
  - Multiply by 0.5: $0.5 \times 25 = 12.5$
  - Divide kinetic energy by product: $100/12.5 = 8$ kg

example 1

$$v^2 = \frac{500j}{0.5 \times 30kg}$$

$$= \frac{500j}{15\ kg}$$

$$v2 = 33.33\ m^2/s^2$$

$$v = \sqrt{33.33\ m^2/s^2}$$

$$v = 5.77 m/s$$

example 1

$$m = \frac{100j}{0.5 \times (5\,m/s)^2}$$

$$= \frac{100j}{0.5 \times 25\ m^2/s^2}$$

$$= \frac{100j}{12.5\ m^2/s^2}$$

$$m = 8\ kg$$

Ex 1

$m = 30 \, kg$

$V = ?$

$KE = 500$

$$KE = \frac{1}{2}mv^2$$

$$\frac{2KE}{m} = v^2$$

$$V = \sqrt{\frac{2 \, KE}{m}}$$

$$V = \sqrt{\frac{2 \times 500}{30}} = 5.773 \, m/s$$

Ex 2

$m = ??$

$V = 5 \, m/s$

$KE = 100 \, J$

$$KE = \frac{1}{2}mv^2$$

$$\frac{2KE}{v^2} = m$$

$$m = \frac{2 \, KE}{v^2} = \frac{2 \times 100}{25} = 8 \, kg$$

Types of Kinetic Energy

There are five types of kinetic energy that are,
•Radiant Energy
•Thermal Energy
•Sound Energy
•Electrical Energy
•Mechanical Energy

• Radiant Energy

Radiant energy is a form of kinetic energy, which is the physical energy of matter resulting from electromagnetic radiation. It is radiated from matter into the surrounding environment.

For example, Ultraviolet light, Gamma rays, and X-rays all have electromagnetic radiant energy.

• Thermal Energy

Thermal energy can be also known as heat energy. It is generated by the kinetic energy of the motion of atoms when they collide with each other.

For Example, Hot Springs, Heated Swimming pools have thermal energy.

أنواع الطاقة الحركية

هناك خمسة أنواع رئيسية من الطاقة الحركية:

.1 الطاقة الإشعاعية (Radiant Energy)

.2 الطاقة الحرارية (Thermal Energy)

.3 الطاقة الصوتية (Sound Energy)

.4 الطاقة الكهربائية (Electrical Energy)

.5 الطاقة الميكانيكية (Mechanical Energy)

1. الطاقة الإشعاعية

• هي شكل من أشكال الطاقة الحركية، وهي الطاقة الفيزيائية للمادة الناتجة عن الإشعاع الكهرومغناطيسي.
• تُشعّ من المادة إلى البيئة المحيطة.
• أمثلة: الضوء فوق البنفسجي، أشعة غاما، الأشعة السينية (X-rays).

2. الطاقة الحرارية

• تُعرف أيضًا بطاقة الحرارة.
• تنتج من الطاقة الحركية لحركة الذرات عند تصادمها مع بعضها البعض.
• أمثلة: الينابيع الساخنة، وأحواض السباحة المُسخنة.

- **Sound Energy**

Sound energy is the energy, produced by the vibration of an object. It travels through the medium but cannot travel in a vacuum or space.

For Example, Tuning Forks, Beating Drums have sound energy.

- **Electrical Energy**

Electrical energy can be obtained from the free electrons that are of positive and negative charge.

For Example, Batteries have electrical energy.

- **Mechanical Energy**

The sum of kinetic energy and potential energy is called mechanical energy. It can neither be created nor destroyed but it can be converted from one form to other.

For Example, Satellites orbiting around the Earth, Moving Cars all have mechanical energy.

3. الطاقة الصوتية (Sound Energy)
- هي الطاقة الناتجة عن اهتزاز جسم ما.
- تنتقل عبر وسط مادي (كالهواء أو الماء)، لكنها لا تستطيع الانتقال في الفراغ أو الفضاء.
- أمثلة: الشوكة الرنانة، قرع الطبول.

4. الطاقة الكهربائية (Electrical Energy)
- تُستمد من الإلكترونات الحرة ذات الشحنات الموجبة والسالبة.
- أمثلة: البطاريات تمتلك طاقة كهربائية.
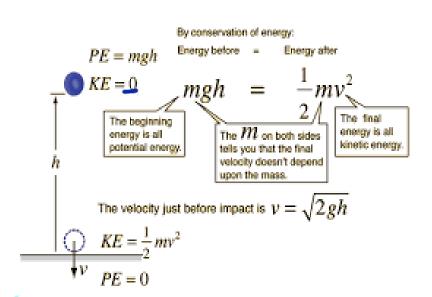
5. الطاقة الميكانيكية (Mechanical Energy)
- هي مجموع الطاقة الحركية والطاقة الكامنة.
- لا تُخلق ولا تُفنى، ولكن يمكن تحويلها من شكل إلى آخر.
- أمثلة: الأقمار الصناعية التي تدور حول الأرض، والسيارات المتحركة.

2-Potential energy

It is the energy resulting from the presence of the body in a specific position, and is often the result of forces The attraction or repulsion of things

Types of potential energy include:

- Gravitational potential energy
- Chemical energy
- Nuclear energy
- Elastic potential energy, also called spring energy

By conservation of energy:

Energy before = Energy after

$PE = mgh$

$KE = 0$

$mgh = \frac{1}{2}mv^2$

The beginning energy is all potential energy.

The m on both sides tells you that the final velocity doesn't depend upon the mass.

The final energy is all kinetic energy.

h

The velocity just before impact is $v = \sqrt{2gh}$

$KE = \frac{1}{2}mv^2$

$PE = 0$

v

الطاقة الكامنة (Potential Energy)

- هي الطاقة الناتجة عن وجود الجسم في موضع معيّن،
- وغالبًا ما تكون نتيجة لقوى الجذب أو التنافر بين الأشياء.

أنواع الطاقة الكامنة تشمل:

1. الطاقة الكامنة الجاذبية (Gravitational Potential Energy):

   ناتجة عن موقع الجسم في مجال الجاذبية.

   مثال: كرة على ارتفاع معيّن عن سطح الأرض.

2. الطاقة الكيميائية (Chemical Energy):

   مخزّنة في الروابط الكيميائية بين الذرات والجزيئات.

   مثال: الغذاء، الوقود.

3. الطاقة النووية (Nuclear Energy):

   ناتجة عن تفاعلات داخل نواة الذرة (انشطار أو اندماج).

   مثال: محطات الطاقة النووية.

4. الطاقة الكامنة المرنة (Elastic Potential Energy) أو طاقة النابض:

   ناتجة عن تمدّد أو انضغاط جسم مرن مثل النابض أو الشريط المطاطي.

   مثال: القوس المشدود، الزنبرك المضغوط.

Gravitational Potential Energy

Gravitational potential energy is the energy stored in an object due to its position above the Earth's surface.
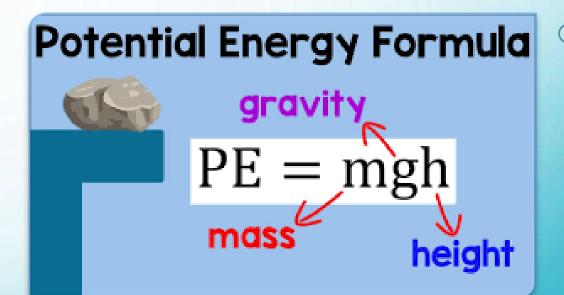
$$PE = E_p = mgh$$

m = mass (kg)

g = gravitational field strength (N/kg) m/s^2

h = height (m)

E_p = gravitational potential energy (J)

Potential Energy Formula

gravity

$$PE = mgh$$

mass   height

Example

A book of mass 1 kg is kept on a library shelf at height. If the change in potential energy is 17. 64J. Then calculate the height of the bookshelf. We already know that the change in energy is equal to the potential energy of the object at that height
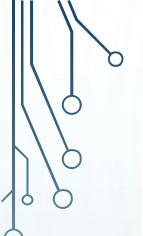
$$\Delta E_{pe} = mgh$$
$$17.64J = 1kg \times 9.8N/kg \times h$$
$$h = \frac{17.64J}{9.8N/kg}$$
$$h = 1.8m$$
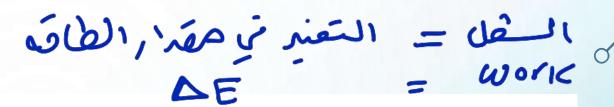
The book is at a height of 1. 8m.

m

n

الحظوا حساب الارتفاع

$$PE = E = \Delta E = mgh$$

$$h = \frac{\Delta E}{mg}$$

PE

$$h = \frac{17.64}{1 \times 9.8} = 1.8m$$

الشغل = التغيير في مقدار الطاقة
work = ΔE

Example

Calculate the work done to raise an object of mass 5.5 Kg to a height of 2.0 m in the earth's gravitational field.

We know that the work done to raise an object to a certain height is the gravitational potential energy of the object at that height so

Mass = 5.50 kg

Height = 2.0 m

$g = 9.8 \text{N/kg}$

$m = 5.5$ $h = 2m$ work

$$Work = \Delta E = mgh = 5.5 \times 9.8 \times 2 = 110 J$$

Substitute these values in the equation for potential energy and we get

$E_{pe} = mgh$

$E_{pe} = 5.50 kg \times 9.8 \text{N/kg} \times 2.0m$

$E_{pe} = 110J$
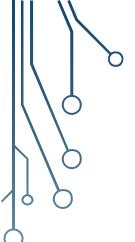
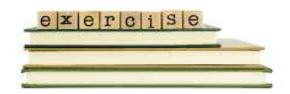Therefore the work done to raise an object of mass 5.5 kg to a height of 2 m is 110J.

Difference Between Kinetic Energy and Potential Energy
The difference between Kinetic Energy and Potential Energy is discussed below,

Kinetic Energy	Potential Energy
Kinetic energy is the energy of any moving object.	Potential energy is the energy of the object due to its position in space.
Formula for kinetic energy is, $$K.E. = 1/2mv^2$$	Formula for potential energy is, $$P.E. = mgh$$
Example: Energy of a moving car.	**Example:** Energy of a book placed on top of the table.

➤ What is potential energy?

Potential energy E$_P$, is a form of energy that depends on the relative position of an object within a system.

➤ What is an example of potential?

❖ ما هي الطاقة الكامنة؟

Examples of potential energy are

الطاقة الكامنة pE هي شكل من أشكال الطاقة التي تعتمد على الموضع النسبي لجسم داخل نظام.

Raised object
Stretched rubber band

❖ ما هي أمثلة على الطاقة الكامنة؟

Water stored in a dam
The energy released during nuclear fusion and fission of atoms

• جسم مرفوع عن سطح الأرض.
• شريط مطاطي مشدود.
• المياه المخزنة في السدود.

➤ What is the formula for calculating potential energy?

• الطاقة المنطلقة أثناء الاندماج أو الانشطار النووي للذرات.

The potential energy can be calculated by EP = mgh

الأنواع الأربعة للطاقة الكامنة هي:

1. الطاقة الكامنة الجاذبية (Gravitational Potential Energy)
2. الطاقة الكامنة المرنة (Elastic Potential Energy)
3. الطاقة الكامنة الكهربائية (Electric Potential Energy)
4. الطاقة الكامنة النووية (Nuclear Potential Energy)

➤ What are the 4 types of potential energy?

The 4 types of potential energy are

Gravitational Potential Energy
Elastic Potential Energy
Electric Potential Energy
Nuclear Potential Energy

◆ ما الفرق بين الطاقة الكامنة والطاقة الحركية؟

• الطاقة الكامنة: هي طاقة مخزنة ناتجة عن الوضع النسبي لجسم داخل نظام.
• الطاقة الحركية: هي طاقة مرتبطة بحركة الجسم.

➤ What is the difference between potential and kinetic energy?

Potential energy is a stored form of energy due to the relative position of an object within a system whereas, kinetic energy is due to the motion of the object

energy ~~power units~~

☐ In the International System of Units SI joules (J)

Where: Joule = Kg.m^2.S^{-2}

$$1J = kg.m^2.s^{-2}$$

$$1J = (kg.m.s^{-2}).m$$

$$1J = N.m$$

☐ In quantum chemistry, we usually use the electron volt (eV)

Power   (energy) الطّاقة

وحدات القياس

$\boxed{\text{جول}}$ $J = \dfrac{kg\, m^2}{s^2} = kg\, m^2\, s^{-2}$

$J = N \cdot m$

$\boxed{\begin{array}{c}\text{الكترون فولت}\\ eV\end{array}}$ $1eV = 1.602 \times 10^{-19}\, J$

$$eV \underset{\div}{\overset{\times\ 1.602\times10^{-19}}{\rightleftarrows}} J$$

$\boxed{\begin{array}{c}calorie\\ \text{كالوري}\end{array}}$ $1\,cal = 4.184\, J$

$$Cal \underset{\div}{\overset{\times\ 4.184}{\rightleftarrows}} J$$

eV **An electron volt** :is the energy obtained by an electron when it passes under the influence of a voltage of one volt (1V).

ا فولت
ضنه الكترون ٩
كولوم

$$1 \text{ eV} = 1.602 \times 10^{-19} \text{ coulomb} \times 1V$$

$$= 1.602 \times 10^{-19} \text{ CV} = 1.602 \times 10^{-19} \text{ J}$$

$$J = eV = \text{منولت . كولوم}$$
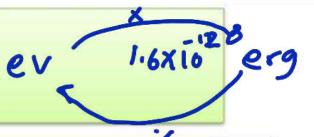
❑ Another commonly used unit is calorie (cal).

حجم الطاقة اللازمة لرفع درجة حرارة عرام
واحد من الماده درجه سلسيوس واحده

Calorie:
It is defined as the amount of energy needed to increase the temperature of one gram of water by one degree Celsius

1 cal = 4.184 J

Units of Energy

ev $\overset{\times}{\underset{\%}{\longleftrightarrow}}$ 1.6×10^{-12} erg

1. ERG – a unit of energy (the smallest unit of energy)
2. ELECTRON VOLT (eV) $1\ eV = 1.60 \times 10^{-12}\ ergs$

(the eV is smaller than the erg, but it is a relative unit whose value must be determined experimentally.)

3. CALORIE – the most commonly used unit of energy.

$$1\ Cal = 4.18 \times 10^7\ ergs$$

4. JOULE - $1\ Joule = 1.00 \times 10^7\ ergs$

$$4.18\ Joules = 1\ Calorie$$

Waves and Particles

In classical physics, the concepts of waves and particles are mutually exclusive.

Waves

الموجات

Wavelength   Frequency

Pass through each other

- Spread in space and time.

تداخل

- Can be superposed – show interference effects.

تداخل

يمكن كلاسكيه

Particles

الجسيمات

- Localized in space and time.

- Cannot pass through each other - they bounce or shatter.

In classical physics, nothing can be both a particle and a wave at the same time.

الفيزياء الكلاسيه سينخيل ان لكون كرة موجه و جسم سويا

➤ Properties of waves

The five important properties of waves are Amplitude, Frequency, Wavelength, period, and Speed. Listed below is a detailed view of all the properties.

1.Amplitude Amplitude is among the first properties of waves and is denoted by the symbol 'A,'.
•Its S.I. unit is a meter (m).

2.Frequency
The second property of waves is the frequency denoted by the symbol 'f.' The Greek symbol is lambda (v), called nu.
•Its S.I. unit is Hertz (Hz), named in honour of a German Physicist – Heinrich Rudolf Hertz.
•It measures the total number of waves passing through a definite point in a given period.
•Frequency is **inversely** proportional to the period and is given by the formula f=1/T.
•The relation between wavelength, speed, and frequency can be determined by λ.
•In the case of an electromagnetic wave that propagates via vacuum, the u is replaced by c (speed of light), and the formula changes to f=c/ λ.

خصائص الموجات ⤝

الخصائص الخمس المهمة للموجات هي: السعة (Amplitude)، التردد (Frequency)، الطول الموجي (Wavelength)، الزمن الدوري (Period)، والسرعة (Speed). فيما يلي عرض تفصيلي لكل خاصية:

1. السعة (Amplitude)
• السعة من أولى خصائص الموجات، ويرمز لها بالرمز A.
• وحدتها في النظام الدولي للوحدات (SI) هي المتر (m).

2. التردد (Frequency)
• الخاصية الثانية من خصائص الموجات هي التردد، ويرمز له بالرمز f.
• الرمز الإغريقي المستخدم هو v (نيو nu).
• وحدته في النظام الدولي للوحدات (SI) هي الهرتز (Hz)، سُمّيت تكريمًا للفيزيائي الألماني هاينريش رودولف هرتز.
• التردد يقيس عدد الموجات الكلي التي تمر عبر نقطة معينة خلال فترة زمنية محددة.
• التردد يتناسب عكسيًا مع الزمن الدوري، ويُعطى بالعلاقة: f = 1/T.
• العلاقة بين الطول الموجي والسرعة والتردد تُعطى بالصيغة: f = v/λ.
• في حالة الموجات الكهرومغناطيسية التي تنتشر في الفراغ، تُستبدل v بـ c (سرعة الضوء)، وتصبح الصيغة: f = c/λ.

3.Wavelength

The wavelength is the third property of waves. It is the total displacement or distance between two corresponding troughs or crests.
- It is denoted by the Greek symbol lambda (λ)
- Its S.I. unit is a meter (m)

4.Time period

- The time period is the fourth property of waves and is defined as the time a particle of a medium takes to make a whole vibrational cycle.
- Its S.I unit is seconds (s)
- The frequency and time period are **inversely** related, T=1/f; if frequency increases, the time period decreases, T represents the time period, and f denotes frequency.

5.Speed/Velocity

- Speed id, the fifth property of a wave, is defined as the total distance covered by a point on the wave in a specific period of time.
- The S.I. unit of speed is metres per second (m/s).
- It depends on the medium through which the wave is propagating.
- The formula for calculating the speed of a wave is speed = Wavelength × frequency.

$$u = \lambda \, \gamma$$

<div dir="rtl">

3. الطول الموجي (Wavelength)
- الطول الموجي هو الخاصية الثالثة للموجات. وهو المسافة الكلية بين قمتين متتاليتين أو قاعين متتاليين للموجة.
- يُرمز له بالرمز الإغريقي λ (لامبدا).
- وحدته في النظام الدولي للوحدات (SI) هي المتر (m).

4. الزمن الدوري (Time Period)
- الزمن الدوري هو الخاصية الرابعة للموجات، ويُعرّف بأنه الزمن الذي يستغرقه جسيم من الوسط لإكمال دورة اهتزازية كاملة.
- وحدته في النظام الدولي للوحدات (SI) هي الثواني (s).
- العلاقة بين التردد والزمن الدوري عكسية: T = 1/f.
- إذا زاد التردد قلّ الزمن الدوري. حيث T يمثل الزمن الدوري و f يمثل التردد.

5. السرعة/السرعة الموجية (Speed / Velocity)
- السرعة هي الخاصية الخامسة للموجات، وتُعرّف بأنها المسافة الكلية التي يقطعها نقطة على الموجة خلال فترة زمنية محددة
- وحدتها في النظام الدولي للوحدات (SI) هي متر لكل ثانية (m/s).
- تعتمد على الوسط الذي تنتشر خلاله الموجة.
- الصيغة الرياضية لحساب سرعة الموجة هي:
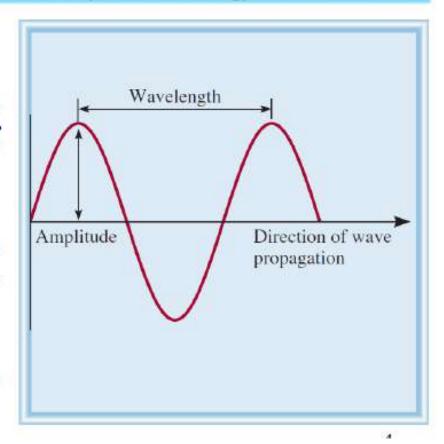- السرعة = الطول الموجي × التردد

</div>

Properties of Waves

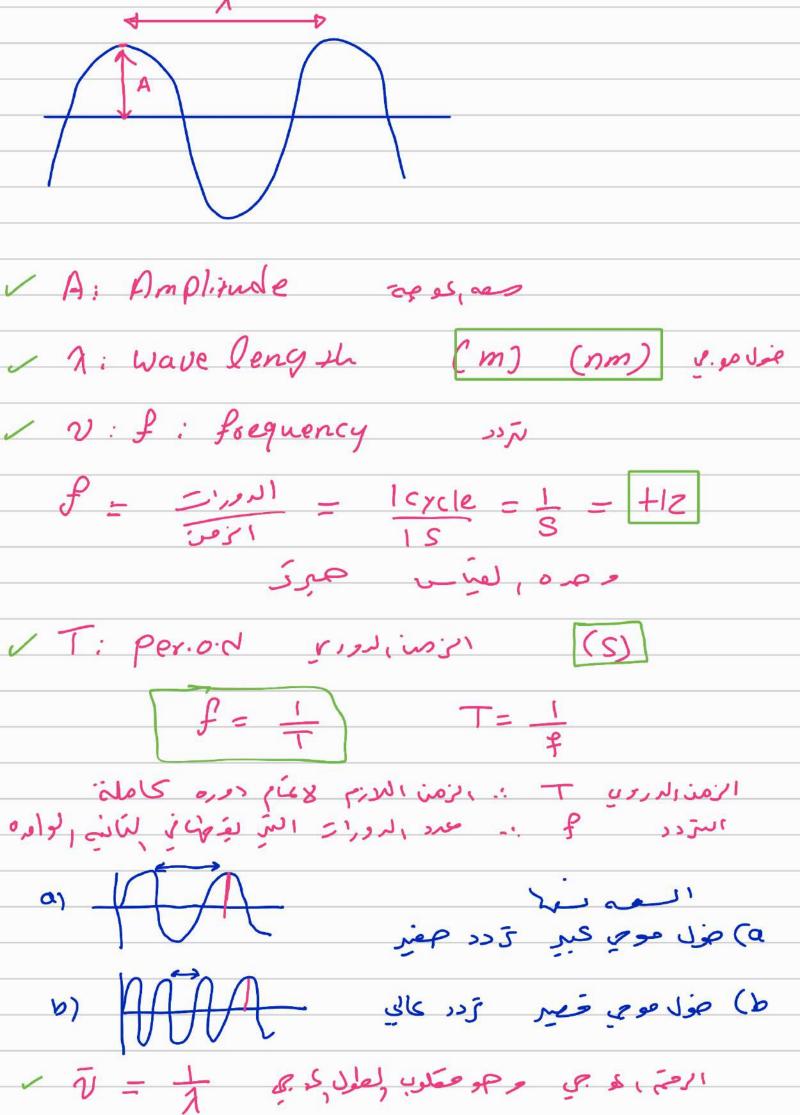A **wave** can be thought of as *a vibrating disturbance by which energy is transmitted.*

Wave characteristics

Wavelength λ (lambda) is the distance between identical points on successive waves.

Frequency v (nu) is the number of waves that pass through a particular point in one second.

Amplitude is the vertical distance from the midline of a wave to the peak or trough.

✓ A: Amplitude   سعة، موجة

✓ λ: wave length   طول موجي   (m) (mm)

✓ ʋ : f : frequency   تردد

$$f = \frac{\text{الدورات}}{\text{الزمن}} = \frac{1\,cycle}{1\,s} = \frac{1}{s} = Hz$$

وحده، لقياس   حبرك

✓ T : period   الزمن، الدور   (S)

$$\boxed{f = \frac{1}{T}} \qquad\qquad T = \frac{1}{f}$$

الزمن الدوري T .. الزمن اللازم لعمل دوره كاملة
التردد f .. عدد الدورات التي يقطعها في الثاني الواحده

a)   السعه نفسها

a) طول موجي كبير   تردد صغير

b)   b) طول موجي قصير   تردد عالي

✓ $\bar{\nu} = \frac{1}{\lambda}$ الرقم، الموجي وهو مقلوب لطول، دي جي

العلاقة بين الطول الموجي و التردد علاقة طردية

$$u = \lambda \nu$$

$u \Rightarrow (m/s)$ سرعة موجه

$u = \lambda u \qquad \lambda = \dfrac{u}{\nu} \qquad \nu = \dfrac{u}{\lambda}$

في حالة الموجات الكهرومغناطيسية (ضوء) سرعة موجه ثابته

$$u = C = 3 \times 10^{8} \ m/s$$

$$C = \lambda \nu$$

طاقة الموجات الكهرومغناطيسية

$$E = h\nu \longrightarrow \text{تردد} \ Hz$$

ثابت بلانك   طاقة J

$$h = 6.626 \times 10^{-34} \ J \cdot s$$

$$\boxed{E = h\nu = \dfrac{hc}{\lambda} = hc\bar{\nu}}$$

The speed of a wave depends on the type of wave and the nature of the medium through which the wave is traveling (for example, air, water, or a vacuum).

The **speed (u) of a wave** is the product of its wavelength and its frequency:
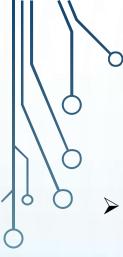
$$u = \lambda\, v$$

Wavelength is usually expressed in units of **meters**, **centimeters**, or **nanometers**, and frequency is measured in **hertz (Hz)**, where

$$1\ Hz = 1\ cycle/s$$

Two waves having different wavelengths and frequencies. The wavelength of the top wave is three times that of the lower wave, but its frequency is only one-third that of the lower wave. Both waves have the same speed and amplitude.

$\bar{\nu}$ مقلوب٢   m

- Wave number: is the reciprocal of the wavelength and is denoted by the symbol $\overline{\nu}$

➤ Its units are the reciprocal of units of length and is defined as the number of waves in 1 meter

- Energy: It is calculated from the relationship

$$E = h\nu$$

$$h = 6.626 \times 10^{-34} \, J \cdot s$$

Where h : Planck's constant is equal to

The relationship between the previous properties

$$E = h\nu = \frac{hc}{\lambda} = hc\,\overline{\nu}$$

$\lambda = 550 \times 10^{-9}\ m$

$C = 3 \times 10^{8}\ m/s$

a) $E = \frac{hc}{\lambda} = \frac{6.626 \times 10^{-34} \times 3 \times 10^{8}}{550 \times 10^{-9}} = 3.164 \times 10^{-19}\ J$

Application:

b) $\nu = \frac{c}{\lambda} = \frac{3 \times 10^{8}}{550 \times 10^{-9}} = 5.45 \times 10^{14}\ Hz$

A sodium lamp emits a yellow light of wavelength   550 nm ?

Calculate E , ν and $\overline{\nu}$

c) $\overline{\nu} = \frac{1}{\lambda} = \frac{1}{550 \times 10^{-9}} = 1.812 \times 10^{6}\ m^{-1}$

❑ Convert wavelength to metre

$\lambda = 550 \text{ nm} = 550 \times 10^{-9} \text{ m} = 5.5 \times 10^{-7} \text{ m}$

$$1 \text{nm} = 10^{-9} \text{ m}$$

1- the wave number (equal to the reciprocal of the wavelength)

$$\overline{\nu} = \frac{1}{\lambda} = \frac{1}{5.5 \times 10^{-7} \text{ m}} = 1.82 \times 10^{6} \text{m}^{-1}$$

2-Frequency:
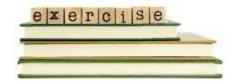
$$\nu = \frac{c}{\lambda} = c\bar{\nu} = 3 \times 10^8 \, \text{ms}^{-1} \times 1.82 \times 10^6 \, \text{m}^{-1} = 5.45 \times 10^{14} \, \text{s}^{-1}$$

3- energy:

$$E = h\nu = 6.626 \times 10^{-34} \, \text{Js} \times 5.45 \times 10^{14} \, \text{s}^{-1} = 3.61 \times 10^{-19} \, \text{J}$$
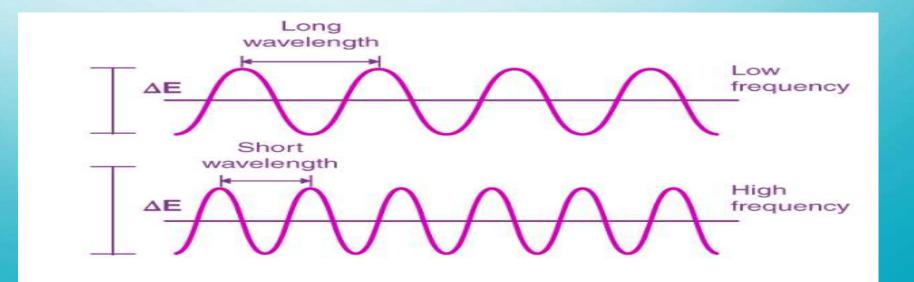
What is the frequency?
Frequency is defined as the number of oscillations of a wave per unit of time and is measured in hertz (Hz)
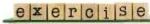
What is a wavelength?
Wavelength is defined as the distance between two nearest points in phase with each other.

What is the relationship between frequency and wavelength? *inverse relation*
The wave speed is equal to the product of its frequency and wavelength.
$V = f \lambda$

$u = f \lambda$

$$C = 3 \times 10^6$$

A radio station broadcasts at a frequency of $99,500,000 Hz$. If the broadcast is an <u>electromagnetic</u> wave, then what is its wavelength?

$$c = 3 * 10^8 \frac{m}{s}$$

$$\lambda = \frac{C}{f} = \frac{3 \times 10^8}{99500000} = 3.02 \, m$$

Explanation:
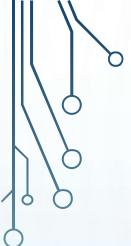
The relationship between wavelength and frequency is given by the equation $\lambda = \dfrac{c}{f}$, where λ is the wavelength, c is the speed of light,

and f is frequency.

We are given the values for frequency and the speed of light, allowing us to solve for the wavelength.

$$\lambda = \frac{c}{f}$$

$$\lambda = \frac{3 * 10^8 \frac{m}{s}}{99,500,000 Hz}$$

$$\lambda = 3.02m$$

A wave oscillates with a speed of $8.9\frac{m}{s}$ and has a wavelength of $6.7m$. What is the frequency of the wave?

$$f = \frac{u}{\lambda} = \frac{8.9}{6.7} = 1.33 \text{ Hz}$$

Explanation:

The equation for velocity in terms of wavelength and frequency is $v = \lambda f$.

We are given the velocity and the wavelength. Using these values, we can solve for the frequency.

$v = \lambda f$

$8.9\frac{m}{s} - 6.7m * f$

$\frac{8.9\frac{m}{s}}{6.7m} = f$

$1.33 Hz = f$

Example

$$T$$

A sound wave has a time period of 0.0001 seconds. What is its frequency?

Answer
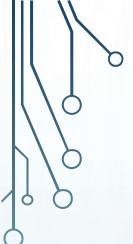
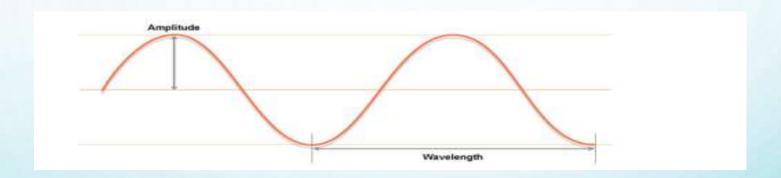$f = \frac{1}{T}$

$f = \frac{1}{0.0001 \text{ s}}$
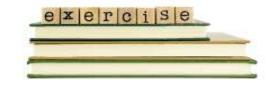
f = 10,000 Hz

The frequency of the sound wave is 10,000 Hz.

$$f = \frac{1}{T} = \frac{1}{0.0001}$$

$$= 10000 \text{ Hz}$$

Sketch a diagram of a wave and label the amplitude and wavelength.

Q1. What is the relationship between frequency and wavelength? (Direct or Inverse)

Q2.What is the relationship between frequency and energy? (Direct or Inverse)

What Is Light?

There was a long debate about the nature of light This debate over the particle or wave nature of light came to a resolution in 1803 when the experiment confirmed that light propagates in waves

﴾ ما هو الضوء؟

كان هناك جدل طويل حول طبيعة الضوء، هل هو ذو طبيعة جسيمية أم موجية.

وقد حُسم هذا الجدل في عام 1803 عندما أثبتت التجارب أن الضوء ينتشر على شكل موجات.

1- الطبيعة الموجية للضوء

الإشعاع الكهرومغناطيسي

1-The Wave Nature of Light

الاشعاع الكهرومغنطير

- الإشعاع الكهرومغناطيسي هو أحد أشكال الطاقة.
- ووفقًا للنظرية الكهرومغناطيسية التقليدية، فإن الطاقة الكهرومغناطيسية تُحمَل بواسطة موجات.
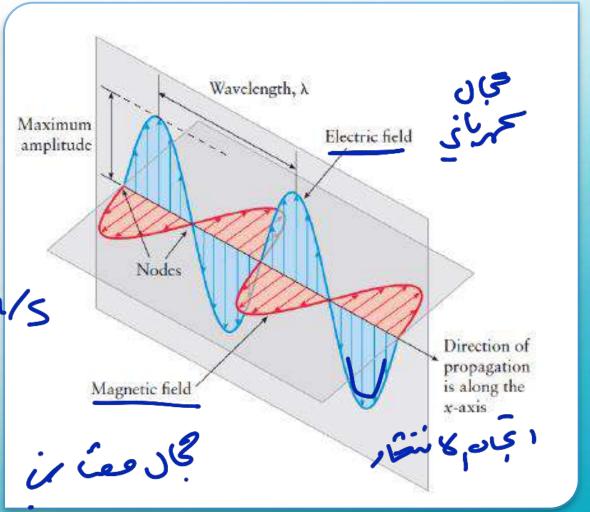- وتنقل هذه الموجات الطاقة في اتجاه انتشارها.
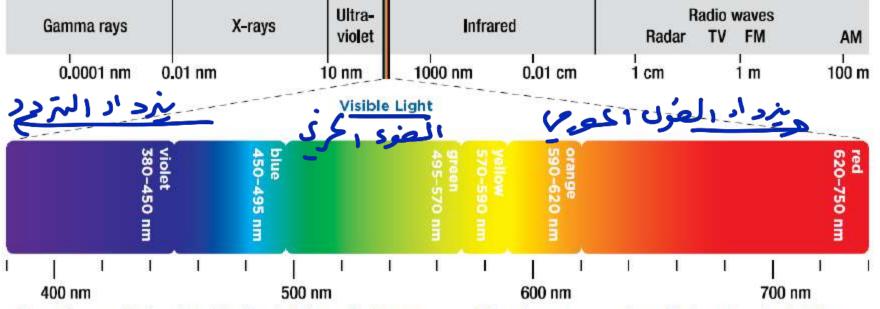
Electromagnetic Radiation

Electromagnetic radiation is one of the forms of energy, and based on the traditional electromagnetic theory, electromagnetic energy is carried by waves and transfers energy in the direction of wave propagation
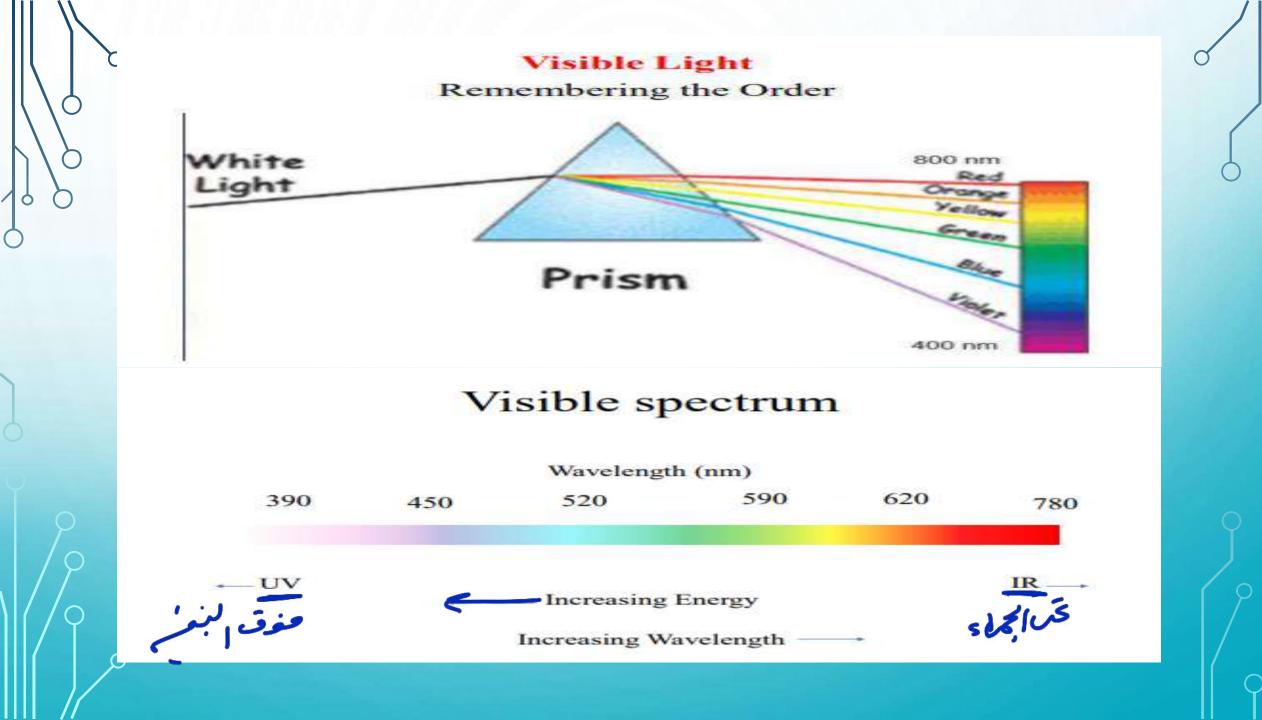
الموجات الكهرومغناطيسيه تتزل في الفراغ

- Electromagnetic waves travel through a <u>vacuum</u> at a constant speed called the <u>speed of light, c</u> which has the defined value of exactly $2.99792458 \times 10^8 \text{ m s}^{-1}$.
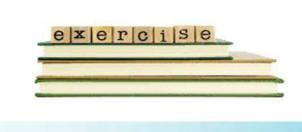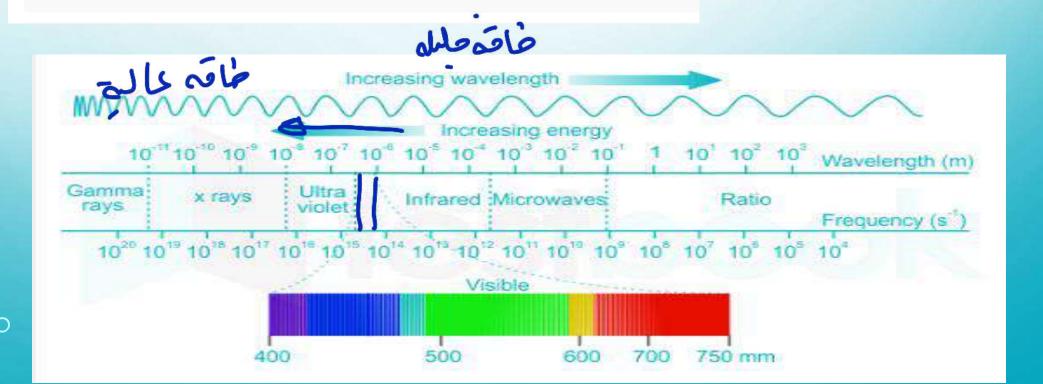
$$C = 2.9979 \times 10^8 \text{ m/s}$$

مجال كهربائي

اتجاه الانتشار

مجال مغناطيسي

الطيف الكهرومغناطيسي

The Electromagnetic Spectrum

Gamma rays	X-rays	Ultra-violet	Infrared	Radio waves Radar TV FM AM
0.0001 nm	0.01 nm	10 nm	1000 nm	0.01 cm	1 cm	1 m	100 m

يزداد التردد ← الضوء المرئي → هيزداد الطول الموجي

Visible Light

violet 380-450 nm
blue 450-495 nm
green 495-570 nm
yellow 570-590 nm
orange 590-620 nm
red 620-750 nm

400 nm — 500 nm — 600 nm — 700 nm

Note the small fraction that is visible to the human eye. The electromagnetic radiation that is visible to the human eye has a wavelength in the range 380 nm (violet light) to 750 nm (red light).

10

Which of the following wave has minimum energy?

1. Radio waves

2. UV rays

3. Infra-red

What is the relationship between frequency and wavelength?

Frequency and wavelength are inversely related. If the wavelength is longer, the frequency is less. A shorter wavelength has a greater frequency.

What is the relationship between frequency and energy?

They are proportionally related. As one becomes greater, so does the other. Energy of a wave is measured by its frequency.
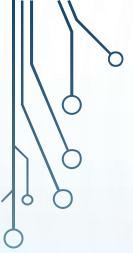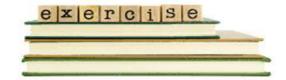
What is the relationship between wavelength and energy?

They are inversely related. Because energy is measured using frequency, and wavelength is inversely related to frequency; this means that wavelength and energy are also inversely related. As wavelength gets longer, there is less energy.

$$E = h\nu$$

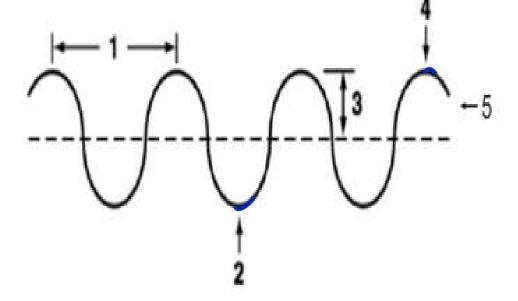| النتيجة	الصيغة/الوصف	العلاقة
كلما زاد الطول الموجي ← قل التردد، وكلما قصر الطول الموجي ← زاد التردد	$\nu \propto \dfrac{1}{\lambda}$	التردد ↔ الطول الموجي
كلما زاد التردد ← زادت الطاقة، وكلما قل التردد ← قلت الطاقة	$E \propto f$	التردد ↔ الطاقة
كلما زاد الطول الموجي ← قلت الطاقة، وكلما قصر الطول الموجي ← زادت الطاقة	$E \propto \dfrac{1}{\lambda}$	الطول الموجي ↔ الطاقة

Label the parts of a wave using the terms: crest, trough, frequency, wavelength, amplitude

1. wavelength

2. trough

3. amplitude

4. crest

5. frequency

2-Particle Nature of Light   الطبيعه الجسيمه للضوء

Classical Physics

In the first half of the 19th century, many discoveries ware made such as:

- Three laws of motion (mechanics) by Newton.

- Three laws of thermodynamics by Rumfold, Joule, Gibbs and Carnot.

- Kinetic theory of gases and statistical mechanics by Maxwell, Gibbs and Boltzmann.

- Wave theory of light by Huygen.

- Optics by Young and Frensel.

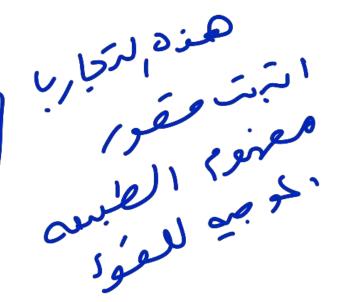The body of these accomplishme

what we now call **classical phys**

خروج علم الكلاسيكية

٢- الطبيعة الجسيمية للضوء

الفيزياء الكلاسيكية

- في النصف الأول من القرن التاسع عشر، تم القيام بالعديد من الاكتشافات مثل:

- قوانين الحركة الثلاثة (الميكانيكا) بواسطة نيوتن.

- القوانين الثلاثة للديناميكا الحرارية بواسطة رمفورد، جول، جيبس، وكارنو.

- النظرية الحركية للغازات والميكانيكا الإحصائية بواسطة ماكسويل، جيبس، وبولتزمان.

- النظرية الموجية للضوء بواسطة هويجنز.

- علم البصريات بواسطة يونغ وفريسنل.

- تُعتبر مجموعة هذه الإنجازات في الفيزياء هي الأساس لتطور ما نُسميه الآن بـ الفيزياء الكلاسيكية.

- By the turn of the 19th century it was pretty much established that **light was an electromagnetic wave**.

- However, three crucial experiments showed that this description of light was incomplete.

- This first was **Blackbody Radiation** (thermal radiation of hot objects).

- The second was the **Photoelectric Effect**.

- The third one was the **Compton Effect**.

هذه التجارب اثبتت قصور مفهوم الطبيعة الموجية للضوء

- مع بداية القرن التاسع عشر، كان قد تم إثبات أن الضوء موجة كهرومغناطيسية بشكل كبير.
- لكن، ثلاث تجارب أساسية أظهرت أن هذا الوصف للضوء غير مكتمل:
  1. إشعاع الجسم الأسود (الإشعاع الحراري للأجسام الساخنة).
  2. التأثير الكهروضوئي.
  3. تأثير كومبتون.

Important Mathematical Foundations in Quantum Chemistry

In our study of quantum chemistry we will encounter some related terms Certain meanings, the most important of these terms are:

1 - differential   2 - Integration   3 - Complex numbers

4 - Vector   5 - Operators   6 - conservative functions

7 - odd and even functions   8 - Reference systems

الأسس الرياضية المهمة في الكيمياء الكمية

في دراستنا للكيمياء الكمية سنواجه بعض المصطلحات ذات الصلة،

ومن أهم هذه المصطلحات:

1. التفاضل
2. التكامل
3. الأعداد المركبة
4. المتجهات
5. المؤثرات (Operators)
6. الدوال المحافظة
7. الدوال الفردية والزوجية
8. أنظمة الإحداثيات (أنظمة المرجع)

First: the differential

differential rule

differential X^n

$$f(x) = y = x^n$$

$$y' = \frac{dy}{dx} = f'(x)$$

$$nx^{n-1}$$

$$f'(x) = n\, x^{n-1}$$

$$f(x) = 3x^5$$

$$f'(x) = 15x^4$$

$$f(x) = x^2 + 3x + 5$$

$$f'(x) = 2x + 3$$

Some important differential laws (note that a is a constant)

y	y'
$\sin x$	$\cos x$
$\cos x$	$-\sin x$
$\sin 4x$	$4\cos 4x$
$\cos x^2$	$-\sin x^2 (2x)$
e^x	e^x
e^{4x}	$4e^{4x}$

$$\frac{d}{dx}a = 0$$

$$\frac{d}{dx}ax^3 = 3ax^2$$

$$\frac{d}{dx}\sin ax = -a\cos ax$$

$$\frac{d}{dx}e^{-ax^2} = -2ax\,e^{-ax^2}$$

$$\frac{d}{dx}x^2.e^{-ax^2} =$$

$$\frac{d}{dx}a = 0$$

$$\frac{d}{dx}ax^3 = 3ax^2$$

$$\frac{d}{dx}\sin ax = a\cos ax$$

$$\frac{d}{dx}e^{-ax^2} = -2ax\ e^{-ax^2}$$

$$\frac{d}{dx}x^2.e^{-ax^2} = x^2(-2axe^{-ax^2}) + e^{-ax^2}(2x)$$

$$= -2ax^3e^{-ax^2} + 2xe^{-ax^2}$$

قانون مشتقة, لضرب

$$\frac{d}{dx}(f.g) = fg' + f'g$$

$$\frac{d}{dx}\left(x^2 e^{-ax^2}\right)$$

$$= x^2\left[-2ax\,e^{-ax^2}\right] + 2xe^{-ax^2}$$

$$= -2ax^3 e^{-ax^2} + 2xe^{-ax^2}$$

Second: integration

انتكامل

integration rule

The integration of X^n

$$\frac{x^{n+1}}{n+1}$$

$$= \int x^n dx = \frac{X^{n+1}}{n+1}$$

$$= \int x^3 dx = \frac{X^4}{4} + C$$

$$\int \frac{1}{x^3} dx = \int x^{-3} dx = \frac{X^{-2}}{-2}$$

$$= -\frac{1}{2x^2} + C$$

❑ This rule is true for both negative and positive n values

$$\int \frac{1}{x} dx = \ln x + C$$

❑Except n=-1

$$\int \frac{f'}{f} dx = \int \frac{2x}{x^2} dx = \ln x^2 + C$$

Second: integration

Some important laws of integration (note that a is a constant)

$$\int 4\,dx = 4x \qquad \int 4\,dy = 4y$$

$$\int \sin x\,dx = -\cos x + C$$

$$\int \cos x\,dx = \sin x + C$$

$$\int e^x\,dx = e^x$$

$$\int e^{3x} = \frac{e^{3x}}{3}$$

$$\int a\,dx = 5x + C$$

$$\int ax^3\,dx = \frac{ax^4}{4} + C$$

$$\int \sin ax\,dx = -\cos x + C$$

$$\int \cos ax\,dx = \sin x + C$$

$$\int a\,dx = ax + c$$

$$\int ax^3\,dx = a\frac{x^4}{4} = \frac{a}{4}x^4 + c$$

$$\int \sin ax\,dx = -\frac{1}{a}\cos ax + c$$

$$\int \cos ax\,dx = \frac{1}{a}\sin ax + c$$

types of integration

a)Unlimited integration:

The limits of integration are not stated

b)limited integration:

The limits of integration are indicated

$$\int_{2}^{3} 3x^2 \, dx = \frac{3 x^3}{3}$$

$$x^3 \Big]_{2}^{3}$$

$$= (3^3) - (2^3)$$

$$27 - 8 = 19$$

$$\int x^n e^{-ax} \, dx = \frac{n!}{a^{n+1}}$$

$$\int_{0}^{\infty} x^n e^{-ax} \, dx = \frac{n!}{a^{n+1}}, n \rangle -1, a \rangle 0 \qquad \int xe^{ax} \, dx = \frac{e^{ax}}{a}\left(x - \frac{1}{a}\right)$$

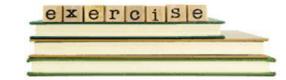$$\int x e^{ax} \, dx = \frac{e^{ax}}{a}\left(x - \frac{1}{x}\right)$$

Application
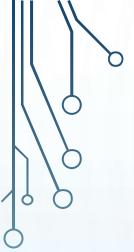
Find the product of the following integrals.

$$\int_1^4 x^2 \, dx = \left. \frac{x^3}{3} \right]_1^4 = \frac{4^3}{3} - \frac{1^3}{3} = \frac{63}{3} = 21$$

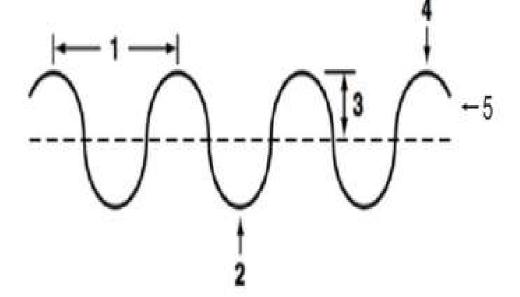$$\int_0^{10} x \, dx = \left. \frac{x^2}{2} \right]_0^{10} = \frac{10^2}{2} - \frac{0^2}{2} = 50$$

$$\int_0^2 e^x \, dx = \left. e^x \right]_0^2 = e^2 - e^0 = e^2 - 1$$

$$21 \cdot 50 (e^2 - 1)$$

$$1050 (e^2 - 1)$$

Label the parts of a wave using the terms: *crest, trough, frequency, wavelength, amplitude*

1. wavelength

2. trough

3. amplitude

4. crest

5. frequency

2-Particle Nature of Light

Classical Physics

In the first half of the 19th century, many discoveries ware made such as:

- Three laws of motion (mechanics) by Newton.

- Three laws of thermodynamics by Rumfold, Joule, Gibbs and Carnot.

- Kinetic theory of gases and statistical mechanics by Maxwell, Gibbs and Boltzmann.

- Wave theory of light by Huygen.

- Optics by Young and Frensel.

The body of these accomplishments in physics is considered the development of what we now call **classical physics**.

- By the turn of the 19th century it was pretty much established that **light was an electromagnetic wave**.

- However, three crucial experiments showed that this description of light was incomplete.

- This first was **Blackbody Radiation** (thermal radiation of hot objects).

- The second was the **Photoelectric Effect**.

- The third one was the **Compton Effect**.

Important Mathematical Foundations in Quantum Chemistry

In our study of quantum chemistry we will encounter some related terms Certain meanings, the most important of these terms are:
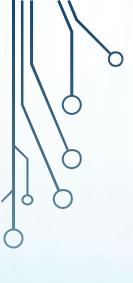
1 - differential

2 - Integration

3 - Complex numbers

4 - Vector

5 - Operators

6 - conservative functions

7 - odd and even functions

8 - Reference systems

First: the differential

differential rule

differential X^n

$$nx^{n-1}$$

Some important differential laws (note that a is a constant)

$$\frac{d}{dx}a$$

$$\frac{d}{dx}ax^3$$

$$\frac{d}{dx}\sin ax$$

$$\frac{d}{dx}e^{-ax^2}$$

$$\frac{d}{dx}x^2 . e^{-ax^2}$$

$$\frac{d}{dx}a = 0$$

$$\frac{d}{dx}ax^3 = 3ax^2$$

$$\frac{d}{dx}\sin ax = a\cos ax$$

$$\frac{d}{dx}e^{-ax^2} = -2ax\ e^{-ax^2}$$

$$\frac{d}{dx}x^2 . e^{-ax^2} = x^2(-2axe^{-ax^2}) + e^{-ax^2}(2x)$$
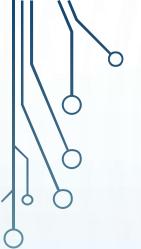
$$= -2ax^3 e^{-ax^2} + 2xe^{-ax^2}$$

Second: integration

integration rule

The integration of X^n

$$\frac{x^{n+1}}{n+1}$$

❑ This rule is true for both negative and positive n values

❑Except n=-1

Second: integration

Some important laws of integration (note that a is a constant)

$$\int a\,dx$$

$$\int ax^3\,dx$$

$$\int \sin ax\ dx$$

$$\int \cos ax\ dx$$

$$\int a\, dx = ax$$

$$\int ax^3\, dx = a\frac{x^4}{4} = \frac{a}{4}x^4$$

$$\int \sin ax\ dx = -\frac{1}{a}\cos ax$$

$$\int \cos ax\ dx = \frac{1}{a}\sin ax$$

types of integration

a)Unlimited integration:

The limits of integration are not stated

b)limited integration:

The limits of integration are indicated

$$\int_{0}^{\infty} x^n e^{-ax} \, dx = \frac{n!}{a^{n+1}}, n \rangle -1, a \rangle 0 \qquad \int xe^{ax} \, dx = \frac{e^{ax}}{a}\left(x - \frac{1}{}\right)$$

Application

Find the product of the following integrals.

$$\int_{1}^{4} x^2 \, dx$$

$$\int_{0}^{10} x \, dx$$

$$\int_{0}^{2} e^{x} \, dx$$