مفردات منهج كيمياء الكم ك٣٢٣ لطلبة قسم الكيمياء في كلية العلوم

١. مقدمة رياضية.
٢. مقدمة تاريخية في اصول ميكانيك الكم.
٣. فرضيات ميكانيك الكم.
٤. حلول دقيقة لمعادلة شرودنكر .
أ- الجسيم الطليق.
ب- جسيم داخل صندوق .
ت- الدوار الصلد.
ث- المهتز التوافقي البسيط.
ج- ذرة الهيدروجين.
٥. الزخم الزاوي.
٦. طريقة تقريبية في ميكانيك الكم.
أ- نظرية التشويش.
ب- نظرية التغيير.
٧. تركيب الذرات والجزيئات:
أ- ذرات اخرى غير ذرة الهيدروجين (ذرة الهيليوم).
ب- برم الالكترون-قاعدة باولي.
ت- طريقة المجال الثابت الذاتي.
ث- أيون جزيئة جزيئة الهيدروجين.
ج- طريقة الاوربتال الجزيني-جزيئة الهيدروجين.
ح- جزيئات ثنائية الذرات ومتعددة الذرات.

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٢. مقدمة في كيمياء الكم تأليف مثنى شنشل .

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الامتحان الاول الخميس ٢٠١٦/١١/ ٢٠١٦ لان ٢٠١٦/١١/١٧ محتمل الاربعينية

الامتحان الثاني الخميس ٢٠١٦/١٢/٢٢

1. Quantum Mechanic:

It was once though that the motion of the atoms and subatomic particles could be expressed using the law of ***classical mechanics*** introduced in seventeenth century by Issaq Newton, for these laws were very successful at explaining the motion of every objects and planets.(الكواكب) however, towards the end of nineteenth century, experimental evidence accumulated showing that classical mechanics failed when it was applied to very small particles and it took until 1920s to discover the appropriate concepts and equations for describing them. We described the concepts of this new mechanics, which is called ***quantum mechanics.***

Quantum mechanics is a branch of science that deals with atomic and molecular properties and behavior of matter on a microscopic scale. While, thermodynamics may be concerned with the heat capacity of a gaseous sample, quantum mechanics is concerned with the specific changes in rotational energy states of the molecules. Chemical kinetics may deal with the rate of change of one substance into another, but quantum mechanics is concerned with the changes in vibrational states and structures of the reactant molecules as they are transformed.

Quantum mechanics is also concerned with the spins of atomic nuclei and the populations of excited states of atoms. Spectroscopy is based on changes of quantized energy levels of several types. Quantum mechanics is thus seen to merge with many other areas of modern science.
A knowledge of the main ideas and methods of quantum mechanics is important for developing an understanding of branches of science from nuclear physics to organic chemistry.

والتطبيقات الحديثة جذور فيزيائية

The modern applications of quantum mechanics have their roots in the developments of physics around the turn of (end of) the century. Some of the experiments, now almost 100 years old, provide the physical basis for interpretations of quantum mechanics. The names associated with much of this early work (e.g., Planck, Einstein, Bohr, de Broglie) are legendary *(imaginary)* in the realm *(world)* of physics. Their elegant experiments and theories now seem almost common place to even beginning students, but these experiments were at the forefront *(initial)* of scientific development in their time.

2. Mathematical Formulas:

There are different mathematical formulas which are necessary to understand them:

a. **Coordination System**:

There are several types for the coordination systems, three class of them can be explained as in the following:

1. ***Cartesian System***: where the point (**P**) include three axis's x,y,z as shown below:

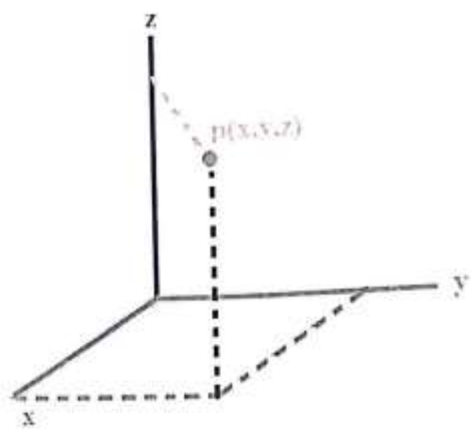


Figure 1: Cartesian coordination system.

All these points lies at:

$-\infty \leq x \leq +\infty$ 1

$-\infty \leq y \leq +\infty$ 2

$-\infty \leq z \leq +\infty$ 3

If the point moves, it varied with respect to time i.e., they behave as a function of time hence:

$d\tau = dxdydz$ 4

Where τ is the volume that surrounded the certain point in space.

Cartesian coordination system is used in case of free particle and particle in box.

2. ***Spherical polar coordination system***: this system can be expressed as the following Figure below:

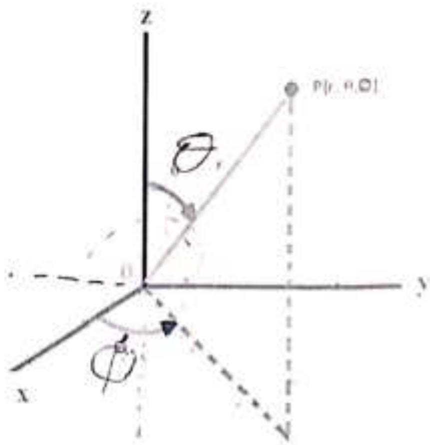


Figure 2: Spherical polar coordination system.

Where the point *(P)* is determined by the arrow r and the two angles θ and $\emptyset$, the long of arrow r is represented by the distance (θP). The angle θ is called ***polar angle*** while, the angle $\emptyset$ is called ***azimuthal angle*** (زاوية السمت) which it lies between x-axis and the projection of *(θP)* in xy plane. The relation between the Cartesian and spherical coordination systems can be explained in the following equations:

$x = r \sin\theta \cos\emptyset$ 4

$y = r \sin\theta \sin\emptyset$ 5

$z = r \cos\theta$ 6

$0 \leq r \leq +\infty$ 7

$0 \leq \theta \leq \pi$ 8

$0 \leq \phi \leq 2\pi$ 9

$d\tau = r^2 \sin\theta \, dr d\theta d\phi$ 10

Spherical coordination system is used for hydrogen atom system.

Home work: proof that: $r^2 = x^2 + y^2 + z^2$ فيثاغورس

3. *Cylindrical coordination system:* the system can be expressed in the following Figure:

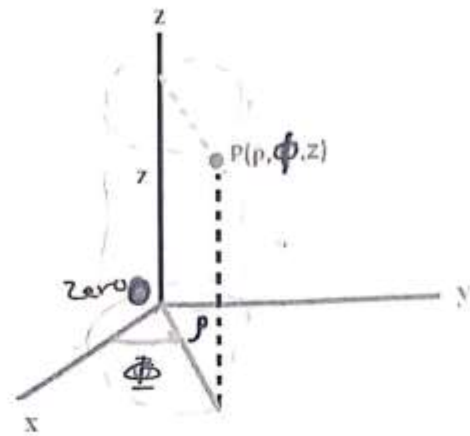


Figure 3: Cylindrical coordination system.

The point p is represented by the two distance ρ and z and the angle Φ which represent the angle between x-axis and the projection of $0p$ (ρ) in xy plane. The relation between Cartesian and cylindrical coordination systems is:

$$x = \rho \cos \emptyset \quad \text{......11}$$

$$y = \rho \sin \emptyset \quad \text{......12}$$

$$z = z \quad \text{......13}$$

$$0 \leq \rho \leq +\infty \text{......14}$$

$$0 \leq \phi \leq 2\pi \text{......15}$$

$$-\infty \leq z \leq +\infty \text{......16}$$

$$d\tau = \rho d\rho d\phi dz \text{......17}$$

The cylindrical system is used for the atoms depending on the problem that it should be solved.

Real Number System:

It is impossible to solve the following equation by using the natural numbers:

$x^2 + 1 = 0$ 18

Thus, the solving of this equation by using the ***imaginary number*** $i = \sqrt{-1}$ (oyler form). Thus, the Gauss form of ***complex numbers*** is

$z = x + iy$..19

The Gauss form is represented by two parts; the first is ***real part (x operator)*** and the second part is ***an imaginary part (y operator)*** where i is the unit of imaginary numbers whereas:

$$i^2 = i.i = -1 \; \& i^3 = i(i^2) = -i \; \& i^4 = (i^2)^2 = 1$$

For each complex number there is consort number z^*:
conjugated

$z^* = x - iy$..20

$z.z^* = (x + iy)(x - iy) = x^2 + y^2$...21

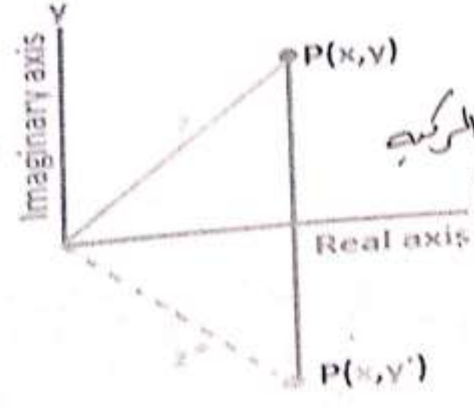
$|z| = \sqrt[2]{z.z^* = (x + iy)(x - iy)} = \sqrt[2]{x^2 + y^2}$..............................22

Equations 24&25 refers to conversion the ***imaginary part*** into ***real part***). Furthermore, all algebraic processes for natural numbers can be used for imaginary numbers for instance:

$z_1 + z_2 = (x_1 + x_2) + i(y_1 + y_2)$ 23

$z_1 - z_2 = (x_1 - x_2) + i(y_1 - y_2)$ 24

Thus, complex number can be represented graphically taking into account the Cartesian system if the real part is x-axis:

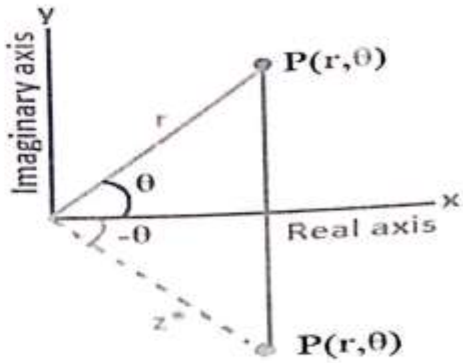


تمثيل الاعداد المركبة بالمحاور الكارتيزية

$z = x + iy$ ……………………………………………………………… 25

$|z| = \sqrt[2]{x^2 + y^2}$ ……………………………………………………… 26

تمثيل الاعداد المركبة بالمحاور القطبية



$x = r\cos\theta$ ……………………………………………………………… 27

$y = r\sin\theta$ ……………………………………………………………… 28

$$z = x + iy = r\cos\theta + ir\sin\theta$$

$z = r(\cos\theta + i\sin\theta)$ …………………………………………………… 29

$z = re^{i\theta}$ ……………………………………………………………… 30

$z^{*} = re^{-i\theta}$ ……………………………………………………………… 31

$$z.z^{*} = re^{i\theta}.re^{-i\theta} = r^2e^{i\theta-i\theta} = r^2$$

$z.z^{*} == r^2$ ……………………………………………………………… 32

$|z| = \sqrt[2]{r^2 = r}$ ……………………………………………………………… 33

Operator:

It can be defines as a series of mathematical process were achieved on a function to convert it into another function that different from each other in their values. If an operator is $O^\wedge$, the function that affected by the particular operator is$O^\wedge F$, the new function is g hence:

$O^\wedge F = g$ ……………………………………………………………… 34

سلسلة من العمليات الرياضية التي تجرى على داله معينة لتحويلها الى داله جديدة تختلف عنها بالقيمة

$O^\wedge$	Original function (F)	Yielded function (g)
C	x	Cx
$\sqrt{\ }$	y	$\sqrt{y}$
$\int_a^b dx$	x	$\frac{1}{2}(b^2 - a^2)$
$\frac{d}{dx}$	$\sin x$	$\cos x$
$\frac{d^2}{dx^2}$	$\sin x$	$-\sin x$

When the symbol (^) is appear in more case i.e. there are different operators, they should be arranged in right form not in wrong e.g.:

$$\alpha^\wedge\beta^\wedge\gamma^\wedge f(x) = \alpha^\wedge\beta^\wedge[\gamma^\wedge f(x)] = \alpha^\wedge\beta^\wedge[f^{\prime}(x)] = \alpha^\wedge[\beta^\wedge[f^{\prime\prime}(x)] = \alpha^\wedge[\beta^\wedge f^{\prime\prime}(x)] = \alpha^\wedge f(x)^{\prime\prime} = f(x)^{\prime\prime\prime} \ldots\ldots 35$$

There are several types for operators some of them are including:

1. **Linear operator:** عندما يشترك المؤثر لعدة دوال لاعطاء نفس النتيجة بعمليات مختلفة تجرى على الدوال بالاثر منفصلة.

It is an operator it is used for different functions to give the same result (superimpose) in different processes that done against the functions in separation manners. The operator is considered a linear if:

$$\alpha^\wedge(f + g) = \alpha^\wedge f + \alpha^\wedge g \ldots\ldots 36$$

$$\alpha^\wedge(af) = a\alpha^\wedge f \ldots\ldots 37$$

There are two types of linear operator includes:

1. $\frac{d}{dx}(f + g) = \frac{df}{dx} + \frac{dg}{dx} \ldots\ldots 38$

While the square root is not considered as an operator because:

$$\sqrt{x + y} \neq \sqrt{x} + \sqrt{y} \ldots\ldots 39$$

2. $\frac{d}{dx}(af) = a\frac{df}{dx} \ldots\ldots 40$

Example 1: The function is f(x) and there are two operators $P^\wedge = \frac{d}{dx}$ & $Q^\wedge = x$ then:

$Q^\wedge P^\wedge f(x) = x\frac{d}{dx}(f) = \frac{xdf(x)}{dx}$ While:

$P^\wedge Q^\wedge f(x) = \frac{d}{dx}([x.f(x)] = \frac{xdf(x)}{dx} + f(x)$ Hence:

$Q^\wedge P^\wedge f(x) \neq P^\wedge Q^\wedge f(x)$ But $(P^\wedge Q^\wedge - Q^\wedge P^\wedge)f(x) = f(x)$

2. **Commutator Operators**:مؤثرات التبادل   اذا كانت المؤثرات متساوية تدعى بالتبادلية

If the two operators are equal then they called as commutator otherwise they not commutators for example if $P^\wedge = \frac{\partial}{\partial x}$ & $Q^\wedge = \frac{\partial}{\partial y}$ then: اي حاصل طرحها = ∅

$P^\wedge Q^\wedge = \frac{\partial}{\partial x}.\frac{\partial}{\partial y} = \frac{\partial^2}{\partial x \partial y}$ & $Q^\wedge P^\wedge = \frac{\partial}{\partial y}.\frac{\partial}{\partial x} = \frac{\partial^2}{\partial x \partial y}$ Thus: $Q^\wedge P^\wedge = P^\wedge Q^\wedge$

$Q^\wedge P^\wedge - P^\wedge Q^\wedge = 0 \leftarrow$ Commutator

$\alpha^\wedge \alpha^\wedge \alpha^\wedge f(x) = \alpha^{\wedge 3} f(x)$ 41

$\frac{d}{dx}.\frac{d}{dx}y(x) = (\frac{d}{dx})^2 y(x) = \frac{d}{dx^2}^2 y(x)$ 42

$\alpha^\wedge.\alpha^{\wedge -1} f(x) = f(x)$ 43

The above is called the ***inverse operator*** or ***unit operator*** (مقلوب المؤثر).

3. Laplacian operator:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \qquad ......44$$

Cartesian coordination(x, y, z)

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}) + \frac{1}{r^2 sin\theta}\frac{\partial}{\partial \theta}(sin\theta\frac{\partial}{\partial \theta}) + \frac{1}{r^2 sin^2\theta}\frac{\partial^2}{\partial \emptyset^2} \qquad ......45$$

Spherical coordination (r, θ, Ø)

$$\nabla^2 = \frac{\partial^2}{\partial \rho^2} + \frac{1}{\rho}\frac{\partial}{\partial \rho} + \frac{1}{\rho^2}\frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2} \qquad ......46$$

Cylindrical coordination (ρ, ϕ, z)

Eigen value equation:

When the operator is used for any function, if the result is the same function multiplied by the constant, the function is called ***Eigen function*** and the factor is called ***Eigen value*** whereas:

$P^{\wedge}F = nF$ 47

Eigen equations are very important in quantum mechanics to solve many problem below table explain the different between Eigen and not Eigen functions:

$O^{\wedge}$	Function	Eigen function or not
$\frac{d}{dx}$	x^2	$2x$ (not)
$\frac{d^2}{dx^2}$	$\sin(n\,x)$	$-n^2\sin x$ ~~(not)~~
$\frac{d}{dx}$	e^{nx}	ne^{nx} (yes)

Example 2: Is the function$\phi(x, y, z) = \sin 2x.\sin 3y.\sin 4z$ is Eigen function? for the operater ∇^2

Solution:

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$\frac{\partial^2}{\partial x^2}(\phi) = -4\sin 2x.\sin 3y.\sin 4z$ 1

$\frac{\partial^2}{\partial y^2}(\phi) = -9\sin 2x.\sin 3y.\sin 4z$ 2

$\frac{\partial^2}{\partial z^2}(\phi) = -16\sin 2x.\sin 3y.\sin 4z$ 3

$$\nabla^2 = -29\underbrace{\sin 2x.\sin 3y.\sin 4z}_{\phi} \neq \phi(x, y, z)$$

Acceptable Function:

There are three condition to be the function an acceptable:

1. It has only one value i.e., it is not curved around itself.
2. It should be continuous

3. The integration of the squared absolute value for the function f(x) should be having a certain value.

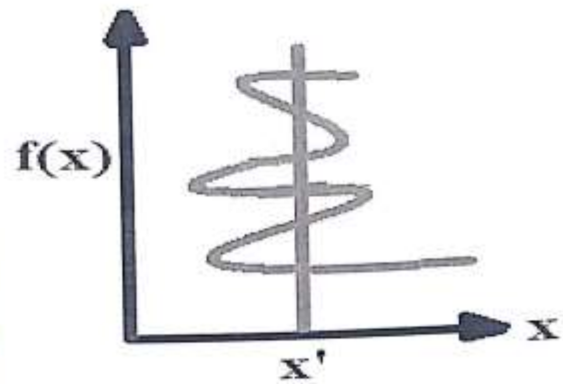


Figure 1: f(x) has five value for f(x) not one value(~~an~~ acceptable).

داله غير مقبولة

Figure 2: f(x) is a contineous function(an acceptable).

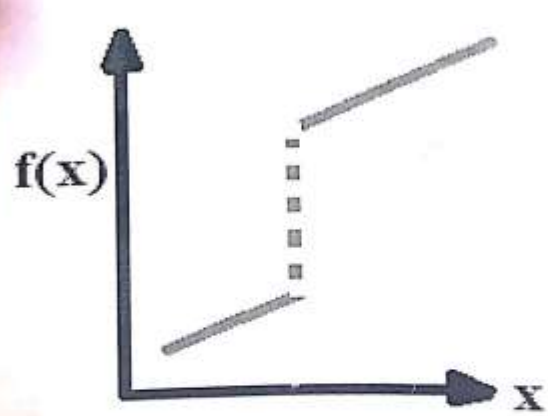


Figure 3: f(x) is not contineous function(not acceptable).

in one dimension

$$F(x) = -\frac{d}{dx}V(x) \quad \text{......52}$$

......53

$$-\frac{d}{dx}V(x) = m\ddot{x} \quad = m\frac{d\dot{x}}{dt} = m\ddot{x}$$

~~If both sides of equation 53 multiplied by dx and integrated:~~

$$\int -dV(x) = m\int \ddot{x}\, dx \quad \text{......54}$$

where $\ddot{x}$ is the acceleration gravity

......55

$$-V(x) + C = \frac{1}{2}m\dot{x}^2$$

Where C is the integration's constant that is time independent. Rearranging of equation 55:

$$C = \frac{1}{2}m\dot{x}^2 + V(x) \quad \text{......56}$$

$$E = T + V(x) \quad \text{......57}$$

Generalized Coordinates and Lagrange& Hamilton kinetic Equations:

To solve the kinetic equation by Newton's law, Cartesian coordinates should be used but the studying of the earth's motion around the sun, the spherical coordinates should be used. Hence, the scientists thought to be found a ***generalized coordinates***. Lagrange and Hamilton are successful to derive the kinetic equations by using the generalized coordinates. It should be understand an idea about the generalized coordinates and the vectorial velocity for conservative system consists of two bodies. Thus, to define the case of like this system, the place and the velocity of both bodies should be determined relative to the time. If the Cartesian coordinate is used then six Cartesian coordinates should be used ($x_1;y_1;z_1; x_2;y_2;z_2$) with six vectorial velocities ($\dot{x}_1;\dot{y}_1;\dot{z}_1; \dot{x}_2;\dot{y}_2;\dot{z}_2$). Generally, for any system include N bodies there are 3N coordinates and 3N vectorial velocities therefore; it has 6N degree of freedom or (degree of changes). If the generalized coordinated is used for N bodies then 3N of generalized coordinates q_i and 3N of $\dot{q}_i$.

$$\dot{q}_j = \frac{dq_j}{dt} \quad \text{(Generalized velocities) ......58}$$

According to generalized coordinates and velocities, the kinetic equations can be derivatives according to Lagrange and Hamilton.

Lagrange equations: Lagrange equation L ($\dot{q}$, q, t) is a scalar dynamic quantity (***non-vectorial dynamic quantity***) is defined by the following equation:

$$-\frac{dV}{dx} = m\ddot{x} = m\frac{d\dot{x}}{dt} \Rightarrow -dV * \frac{dt}{dx} = m\,d\dot{x}$$

$L(q^{\cdot},q,t) = T(q^{\cdot},q) - V(q,t)$ 59

T is the kinetic energy which is the function of generalized coordinates and velocities; (V) is the potential energy which is the function for the generalized coordinates and the time. The general formula for Lagrange equation is:

$$\frac{d}{dt}\left(\frac{\partial L}{\partial q^{\cdot}_j}\right) - \frac{\partial L}{\partial q_j} = 0 \quad \text{.........60}$$

answer (why)

Equation 60 is second order differential equation.

For instance, simple harmonic motion is an applied example for Lagrange equation where the force that re back the oscillator into the start point is directly proportional with the moving of the oscillator from this point. Where the kinetic quantities in this example converted the generalized coordinates into Cartesian coordinates as in below: (q_j, t)

$$q_j = x\,, q^{\cdot}_j = x^{\cdot}\,, T(q_j, q^{\cdot}_j) = \tfrac{1}{2}mx^{\cdot 2}\,, V(q_j) = \tfrac{1}{2}kx^2$$

Applying Lagrange function (q˙, q) according to equation 59:

$$L(x, x^{\cdot}) = \tfrac{1}{2}mx^{\cdot 2} - \tfrac{1}{2}kx^2 \quad \text{.........61}$$

to calculate the kinetic equations:

$$\frac{\partial L}{\partial x^{\cdot}} = mx^{\cdot} \;\&\; \frac{\partial L}{\partial x} = -kx \quad \text{.........62}$$

Substitution of 62 in 60:

$$\frac{d}{dt}(mx^{\cdot}) + kx = 0 \quad \text{.........63}$$

Differential of equation 63:

$$mx^{\cdot\cdot} + kx = 0 \quad \text{.........64}$$

$$mx^{\cdot\cdot} = -kx \quad \text{.........65}$$

F = ma

Equation 65 is same as second newton's law in equation 48.On the other hand:

$$P_i = \frac{\partial L}{\partial q^{\cdot}_i} \quad \text{.........66}$$

Equation 66 represents the generalized momentum $mx^{\cdot}$, $my^{\cdot}$ or $mz^{\cdot}$.

$$\dot{P}_i = \frac{\partial L}{\partial \ldots} \quad \text{.........67}$$

Hamilton's equations:

Hamilton's equation for the certain system include N particles is written as below:

$$\mathcal{H} = \sum_{j=1}^{3N} p_j \dot{q}_j - L \quad \ldots\ldots 68$$

Where H is the Hamilton's function, L is the Lagrange's function, p_j is the generalized momentum and $\dot{q}_j$ is the generalized velocity. It can be derived two equations relative to equation 67 for the conservative system as below:

$$\frac{\partial \mathcal{H}}{\partial p_j} = \dot{q}_j \quad \ldots\ldots 69$$

$$\frac{\partial \mathcal{H}}{\partial q_j} = \frac{-\partial L}{\partial q_j} = -\dot{p}_j \quad \ldots\ldots 70$$

The function H represents the total Energy if the system is conservative which can be prove it by depending on the definition of the generalized momentum according to the equation 59:

$$L(\dot{q}, q, t) = T(\dot{q}, q) - V(q, t) \quad \ldots\ldots 59$$

$$p_j = \frac{\partial L}{\partial \dot{q}_j} = \frac{\partial T}{\partial \dot{q}_j} \quad \ldots\ldots 71$$

Substitution of equations 59&71 into equation 68:

$$\mathcal{H} = \sum_{j=1}^{3N} \dot{q}_j \frac{\partial T}{\partial \dot{q}_j} - T + V \quad \ldots\ldots 72$$

The right limit in the above is equal to 2T. This can be proved as below:

If the certain particle is moved in one dimension. The kinetic energy T can be written relative to the generalized velocity:

$$T = \frac{1}{2} m \dot{q}_j^2 \quad \ldots\ldots 73$$

Differential of equation 73:

$$\frac{\partial T}{\partial \dot{q}_j} = m \dot{q}_j \quad \ldots\ldots 74$$

Multiplied equation 74 by the vectorial velocity $\dot{q}_j$:

$$\dot{q}_j \frac{\partial T}{\partial \dot{q}_j} = m \dot{q}_j^2 = 2T \quad \ldots\ldots 75$$

For many particles are moved in different dimensions, the kinetic energy T:

$$T = \frac{1}{2}\sum_j m\dot{q}_j^2 \quad \dots\dots 76$$

Hence:

$$\sum_j \dot{q}_j \frac{\partial T}{\partial \dot{q}_j} = 2T \quad \dots\dots 77$$

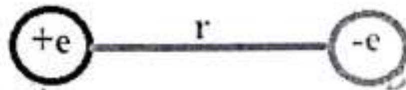
Substitution the above value in equation 72:

$$\mathcal{H} = 2T - T + V = T + V \quad \dots\dots 78$$

As shown above in equation 78 Hamilton's function represents the total energy if the system is conservative.

***Problem* (1):** write the Hamilton's function for hydrogen's and helium's atoms

Solution: for the founding of Hamilton's function for hydrogen atom, it can be assumed the nucleus of hydrogen's atom is constant and there is an electron is moved around the nucleus by the distance equal to r:



نواة

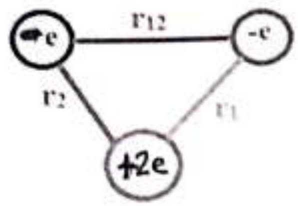
$$T = \frac{1}{2}mv^2 = \frac{m^2v^2}{2m} = \frac{p^2}{2m} \qquad \boxed{mv = p}$$

Where m is the mass of atom and p is the moment. To write the Hamilton's function H which equal to the total of kinetic (T) and potential energy (V) for hydrogen atom:

$$\mathcal{H} = T + V$$

$$\mathcal{H} = \frac{p^2}{2m} + \frac{(+e)(-e)}{r} = \frac{p^2}{2m} - \frac{e^2}{r}$$

For helium's atom the Hamilton's function, assumed that its nucleus is constant, the distance between the nucleus and the first electron is r_1 while the distance between the nucleus and the second electron is r_2 while, the distance between the two electrons is r_{12} then the Hamilton's function for Helium's atom:



$$\mathcal{H} = T + V$$

$$\mathcal{H} = \frac{p_1^2}{2m} + \frac{p_2^2}{2m} - \frac{2e^2}{r_1} - \frac{2e^2}{r_2} + \frac{e^2}{r_{12}}$$

Problem (2): write the Lagrange's and Hamilton's functions for the solid particle has the mass (m) which is moved by a simple harmonic motion to vibrate at distance about (x):

Solution: according to the mentioned functions as the particle is moved as in simple harmonic motion then: 2016-2017

$q = X$ & $q^{\bullet} = x^{\bullet}$ ……1

$T = \frac{1}{2} m x^{\bullet 2}$ ……2

$V = \frac{1}{2} k x^2$ ……3

$L = \frac{1}{2} m x^{\bullet 2} - \frac{1}{2} k x^2$ ……4

$p_x = \frac{\partial L}{\partial x^{\bullet}} = m x^{\bullet}$ ……5

$T = \frac{1}{2} m x^{\bullet 2} = \frac{1}{2} m \left(\frac{p_x}{m}\right)^2 = \frac{p_x^2}{2m}$ ……6

$\mathcal{H} = T + V = \frac{p_x^2}{2m} + \frac{1}{2} k x^2$ ……

Hamilton's and Lagrange's' equations for two attractive particles:

Suppose two attractive particles with the mass m_1 and m_2 respectively. Their potential's energies represent by the distance between them i.e., Their potential's energies represent by their internal coordinate. For instance, if the two-particles are represent by the Cartesian coordinates x_1, y_1, z_1, x_2, y_2 and z_2 the square represented by the Cartesian coordinates distance between them is: 2016-20

$r_{12}^2 = (x_2 - x_1)^2 + (y_2 - y_1)^2 + (z_2 - z_1)^2$ ……79

It can be simplified by using the central's mass coordinates X, Y, Z and the internal coordinates x, y, z. the central's mass coordinates are represented by the following equations:

$$X = \frac{m_1x_1+m_2x_2}{m_1+m_2} \quad \text{......80}$$

$$Y = \frac{m_1y_1+m_2y_2}{m_1+m_2} \quad \text{......81}$$

$$Z = \frac{m_1z_1+m_2z_2}{m_1+m_2} \quad \text{......82}$$

All year 2016-2017

The internal coordinates is represented by:

$$x = x_2 - x_1, y = y_2 - y_1, z = z_2 - z_1 \quad \text{......83}$$

By applying Lagrange's function for this system by more calculations the results are:

$$L = \frac{1}{2}(m_1 + m_2)(\dot{X}^2 + \dot{Y}^2 + \dot{Z}^2) + \frac{1}{2}\mu(\dot{x}^2 + \dot{y}^2 + \dot{z}^2) - V(x, y, z) \quad \text{..84}$$

internal coordinate.

$$\mu = \frac{m_1m_2}{m_1+m_2} \quad \text{......85}$$

Where μ is the reduced mass and V is the potential energy which is depend on the internal coordinates. The kinetic equation can be obtained by using equation 60 from the equation 84: $\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_j}\right) - \frac{\partial L}{\partial q_j} = 0$

$$(m_1 + m_2)\ddot{X} = 0, (m_1 + m_2)\ddot{Y} = 0, (m_1 + m_2)\ddot{Z} = 0 \quad \text{......86}$$

$$\mu\ddot{x} = -\frac{\partial V}{\partial x}, \mu\ddot{y} = -\frac{\partial V}{\partial y}, \mu\ddot{z} = -\frac{\partial V}{\partial z} \quad \text{......87}$$

internal

Equation 86 is same as the motion of free particle with mass that equal to the total of the masses' system which represents the masses' center point. The integration for equation 86 results:

$$(m_1 + m_2)\dot{X} = (m_1 + m_2)\dot{Y} = (m_1 + m_2)\dot{Z} = C \quad \text{......88}$$

Hence, the three vectorial velocities ($\dot{X}$, $\dot{Y}$, and $\dot{Z}$) for the masses' center point is constant and the kinetic energy also should be constant.

On the other hand, equation 87 is same as the motion of free particle with the mass is μ that has a potential energy V(x, y, z) i.e., if V is depended upon the internal coordinates only, the kinetic equations of the central mass can be separated from the kinetic equations of the internal coordinates and solved them separately which simplify the calculations.

Old Quantum theory نظرية الكم القديمة

Blackbody Radiation:

When an object is heated to incandescence *(lightning)* it emits electromagnetic radiation. The nature of the object determines to some extent **(range)** the type of radiation that is emitted, but in all cases a range or distribution of radiation is produced. It is known that the ***best absorber*** of radiation is also the *best emitter* of radiation. The best absorber is a so-called ***"blackbody"*** which *absorbs all radiation* and from which none *is reflected*. If we heat this blackbody to *incandescence*, it will emit a whole range of electromagnetic radiations whose energy distributions depend on the temperature to which the blackbody is heated. Early attempts to explain the distribution of radiation using the ***laws of classical physics*** were *not successful*. In these attempts it was assumed that the radiation was emitted because of ***vibrations*** or *oscillations* within the blackbody. These attempts failed to explain the position of the maximum that occurs in the distribution of radiation; in fact, they failed to predict the maximum at all. Since radiation having a range of frequencies (υ) is emitted from the blackbody, theoreticians tried to obtain an expression that would predict the relative intensity (amount of radiation) of each frequency. One of the early attempts to explain blackbody radiation was made by **W. Wien**. The general form of the equation that Wien obtained is:

$$f(\upsilon) = \upsilon^3 g\left(\frac{\upsilon}{T}\right) \qquad \text{.......... 1}$$

Where $f(\upsilon)$ is the amount of energy of frequency υ emitted per unit volume of the blackbody and $g(\upsilon/T)$ is some function of υ/T. This result gave fair agreement with the observed energy distribution at longer wavelengths but did not give agreement at all in the region of short wavelengths. Another relationship obtained by the use of classical mechanics is the expression derived by **Lord Rayleigh**,

$$f(\nu) = \left(\frac{8\pi\upsilon^3}{c^3}\right) kT \qquad \text{.......... 2}$$

Where c is the velocity of light (3.00×10^8 m/s) and k is Boltzmann's constant, 1.38×10^{-23} J.k^{-1}. Another expression was found by Rayleigh and Jeans predict the shape of the energy distribution as a function of frequency, but only in the region of short wavelengths. The expression is

$$f(\nu) = \left(\frac{8\pi\upsilon^3}{c^3}\right)\left(\frac{hkT}{h\upsilon}\right) = \frac{8\pi\upsilon^2 kT}{c^3} \qquad \text{.......... 3}$$

Therefore, the *Wien relationship* predicted the intensity of high-λ radiation, and the *Rayleigh–Jeans law* predicted the intensity of low λ radiation emitted from a blackbody. Neither of these relationships predicted a distribution of radiation that goes through a maximum at some frequency with smaller amounts emitted on either end of the spectrum.

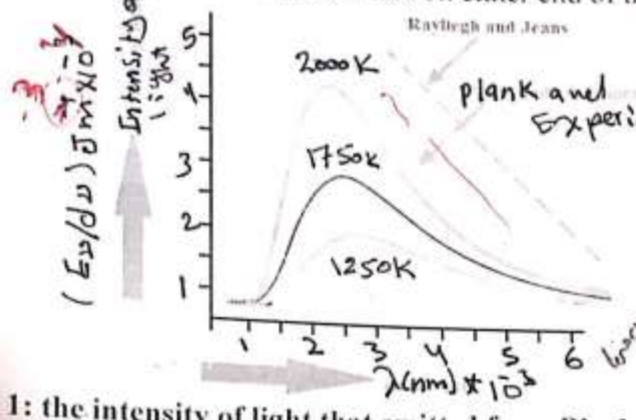


Figure 1: the intensity of light that emitted from Black body radiation at different temperatures relative to Rayleigh and Jeans.

The problem of blackbody radiation was finally explained in a satisfactory way by ***Max Planck*** in 1900. Planck still assumed that the absorption and emission of radiation arose from some sort of oscillators. Planck made a fundamental assumption that only certain frequencies were possible for the oscillators instead of the whole range of frequencies that were predicted by classical mechanics. The permissible frequencies were presumed to be some multiple of a fundamental frequency of the oscillators, ν. The allowed frequencies were then $\nu_0, 2\nu_0, 3\nu_0, \ldots$. Planck also assumed that energy needed to be absorbed to cause the oscillator to go from one allowed frequency to the next higher one and that energy was emitted as the frequency dropped by ν_0. He also assumed that the change in energy was proportional to the fundamental frequency, ν_0. Introducing the constant of proportionality h,

$$E = h\nu_0 \qquad \ldots\ldots 4$$

Where h is Planck's constant, 6.63×10^{-34} J.s. The average energy per oscillator was found to be:

$$\langle E\rangle = \frac{h\nu_0}{(e^{\frac{h\nu_0}{kT}}-1)} \qquad \ldots\ldots 5$$

Planck showed that the emitted radiation has a distribution given by:

$$f(\nu) = \frac{8\pi\nu^3}{C^3}\langle E\rangle = \frac{8\pi\nu^3}{C^3}\frac{h\nu_0}{(e^{\frac{h\nu_0}{kT}}-1)} \qquad \ldots\ldots 6$$

flowing when light was involved became to be known as the *photoelectric effect*. Studying the photoelectric effect involves an apparatus like that shown schematically in Figure 7. An evacuated tube is arranged so that the highly polished metal, such as sodium, potassium, or zinc, to be illuminated is made the cathode. When light shines on the metal plate, electrons flow to the collecting plate (anode), and the ammeter, A, indicates the amount of current flowing. Several observations can be made as the frequency and intensity of the light are varied:

metal plate

Collecting plate

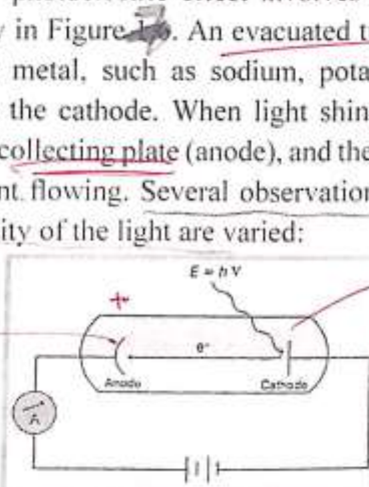


Figure 7: Experimental arrangement for studying the photoelectric effect.

1. The light must have some minimum or threshold frequency, ν, in order for the current to flow.
2. Different metals have different threshold frequencies.
3. If the light striking the metal surface has a frequency greater than ν, the electrons are ejected with a kinetic energy that increases with the frequency of the light.
4. The number of electrons ejected depends on the intensity of the light but their kinetic energy depends only on the frequency of the light.

*An electron traveling toward the collector can be stopped if a negative voltage is applied to the collector. The voltage required (known as the stopping potential, V) to stop the motion of the electrons (causing the current to cease) depends on the frequency of the light that caused the electrons to be ejected. In fact, it is the electrostatic energy of the repulsion between an electron and the collector that exactly equals the kinetic energy of the electron. Therefore, we can equate the two energies by the equation

$$Ve = \frac{1}{2}mv^2 \quad \ldots\ldots 27$$

*An understanding of the photoelectric effect was provided in 1905 by Albert Einstein. Einstein based his analysis on the relationship between the energy of light and its frequency that was established in 1900 by Planck. It was assumed that the light behaved as a collection of particles (called *photons*) and the energy of a particle of light was totally absorbed by the collision with an electron on the metal surface. Electrons are bound to the surface of a metal with an energy called the *work function*, w, which is different for each type of metal.

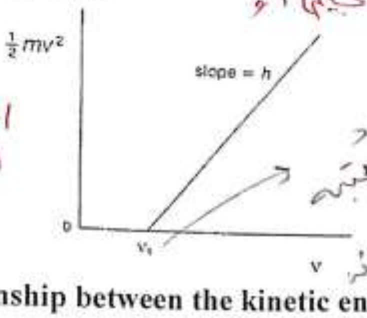


Figure 8: The relationship between the kinetic energy of the ejected electrons and the frequency.

When the electron is ejected from the surface of the metal, it will have a kinetic energy that is the difference between the energy of the incident photon and the work function of the metal. Therefore, we can write

$$\frac{1}{2}mv^2 = hv - w \ldots \Rightarrow \frac{1}{2}mv^2 = hv - hv_0 \ldots\ldots 28$$

It can be seen that this is the equation of a straight line when the kinetic energy of the electron is plotted against the frequency of the light. By varying the frequency of the light and determining the kinetic energy of the electrons (from the stopping potential) a graph like that shown in Figure 7 can be prepared to show the relationship. The intercept is v_o, the threshold frequency, and the slope is Planck's constant h. One of the significant points in the interpretation of the photoelectric effect is that light is considered to be particulate in nature. In other experiments, such as the diffraction experiment of T. Young, it was necessary to assume that light behaved as a wave. Many photovoltaic devices in common use today (light meters, optical counters, etc.) are based on the photoelectric effect.

Particle–Wave Duality

Because light behaved as both waves (diffraction, as proved by Young in 1803) and particles (the photoelectric effect shown by Einstein in 1905), the nature of light was debated for many years. Of course, light has characteristics of both a wave and a particle, the so-called *particle–wave duality*. In 1924, Louis de Broglie, a young French doctoral student,