A COMPUTER PROGRAMME FOR SOLVING REACTION KINETIC AND QUANTUM MECHANICAL PROBLEMS

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NIGER STATE

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TITLE PAGE

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FEDERAL UNIVERSITY OF TECHNOLOGY, MINNA.
NIGER STATE

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APPROVAL PAGE

This is to certify that project is an original work undertaken by MOHAMMED ABDULLAHI and has been prepared in accordance with the regulation governing the preparation, and preparation of project in F.U.T.Minna. This project has been duly supervised and approved by following signatures

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Head of department
Dr.S.A. Reju

Project Supervisor
Mr. Badmus

....

External Examiner

DEDICATION

Dedicated to my parents for their love and kindness.

ACKNOWLEDGEMENT

My sincere appreciation goes to God Almighty who has guided and protect me throughout my course, let honors, glory and power be ascribed unto him forever and ever (Amean).

I also want to thank my humble head of Department Mathematics/Computer science Dr. S.A.Reju who serves as an inspector and model for me. I also wish to extend my portend gratitude to my able co-ordinator PGD Computer Science, Mr. Ezeko and Lecturers in the department as well as my project Supervisor, Mr. Badmos who have helped me in one way or the other.

I also owe dept of gratitude to my grand parents, my parents, brothers and Sisters for their assistance and encouragement that enables me achieve my set down goals and objectives.

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ABSTRACT

This project will be design to give an introduction to the study of computer programme for solving reaction kinetics and Quantum Mechanical Problems.

The project is an introduction to the essential ideas in differential equation rather than a comprehensive account of the subject. It considers some types of reactions, Quantum, classical mechanics, Schrodinger equation and wave equations are considered in the work were calculated.

While in the study of most of differential equations, the tools used are restricted almost completely to algebra, here in this course work one use much of differential calculus and some time integral calculus. Therefore, the work deals essentially with simple reactions of kinetics and Quantum.

In chapter four, one shall be discuss mainly on programming.

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This facts has been known for a long period of time, but Wenzel (1740-1793) Working on the corrosion of metals by acids (1777) was the first to introduce the idea of relationship between the acid concentration and the rate of attach the metal or the weight devolve in unit time.

It was not until or 1850 that Wilhelmy, using the inversion of sugarcane by acid, Showed the proportionality of the reaction rate with the concentration of the reagents.

This becomes the first experimental fact in kinetics although at the time it past almost unnoticed.

Chemical kinetic did not come on its own however, until 1884 with vanthoff (1852-1911) and is classic works. A study of chemical dynamics therefore Vanthoff and Withelmy, can both be considered the true founders of this branch of chemistry.

Up to that time-and one must not forget that the first edition of Mendeleef' speriodic classification of chemistry only appeared in 11870 chemist had restricted themselves to the study of what is easiest in a chemical reaction, that is initial and final state. All of the static characteristics in a chemical reaction are beginning to be properly explored, the reagents the products of the reaction, are all balance the energy involved etc The manner however, in which the reaction took place was completely known, its mechanism and the relationship would have with the reaction rate or with the structure of the different reacting species had not been foreseen nor the dependence of the mechanism on the external condition of temperature, pressure physical rate of the reagent etc.

Thermodynamics, this science which developed long before chemical kinetics, predict whether a reaction will proceed under a given set of conditions of temperature and pressure. It can also predict the direction in which the equilibrium will be shifted in response to a variation in these parameters. However, it can not tell us what the rate of the reaction will be nor how this rate will vary with the significant factors such as temperature pressure composition of the reaction mixture etc.

The Quantum mechanical plays an essential role in our understanding of molecular vibrations. Their spectra, and their influence on thermodynamic properties. The problem provides a good domestication of mathematical techniques that are important in quantum chemistry. Since many chemists are overly familiar with some of the mathematical concepts, one shall deal with them in detail in the context of this problem.

1.2 CLASSIFICATION OF DIFFERENTIAL EQUATION

Differential equation is classified into two main categories- partial and Ordinary differential equation One of the must obvious classifications is based on whether the unknown function depend on a single independent variables or in several independent variable. In the first case only portion derivatives appear is called partial differential equation.

Example $d^2u/dx^2(x,y)+du/dy(x,y)=o$ is called second order partial differential equation.

In the second case only ordinary derivatives appear in the differential equation, and it is said to be an ordinary differential equation.

Example $dR/dt(t)=-kR(t)$ where k is a known constant is called first order ordinary differential equation

(i) $Ld^2\theta(t)/dt^2+Rd\theta(t)/dt+\frac{1}{c}\theta(t)=E(t)$ for the charge $\theta(t)$ on a condenser in a circuit with capacity c, resistance R, inductance L, and impressed voltage E(t), is the example of second order ordinary differential equation.

1.3 ORDER OF DIFFERENTIAL EQUATION

The order differential equation is the order of the high power derivatives

Example-:

(i) $dy/dx+f(x,y)=O$ is called first order differential equation

(ii) $dy/dx+f(x,y)=$ is called first differential equation.

(iii) $d^2y/dx^2+dy/dxp(x)+q(x)y=o$ is called second order differential equation etc

1.4 DEGREE OF DIFFERENTIAL EQUATION

The degree of differential equation is the exponent of the highest power of the highest order derivative.

Example-:

(i) $dy/dx=x/y$ is called differential equation of degree one.

(ii) $dy/dx=(9x^2+2xy+3y^2)/2x(x+y)$ is differential equation of degree two etc

1.5 ORDINARY DIFFERENTIAL EQUATION

If in a differential equation, the dependent variable is a function of only one Independent variable Example $dy/dx=3x+7x+5$

Ordinary differential equation is further classified as linear or non-linear homogenous or non-homogeneous and first order or second order or third order.

A differential equation is said to be linear if each term is linear (degree one or Zero) in term of all dependent variable and their derivatives. For example $dx/dt+x = t^3$ So it is called a non linear differential equation Example $(dx/dt)^2 + dx/dt-x-y=7t$

If in the differential equation the only term consisting entirely of the independent variable is zero, then the differential equation is called a homogeneous differential equation.

An example of homogeneous differential equation is $d^2y/dx^2+xdy/dx+y=0$ An equation that is not homogeneous is called non-homogeneous equation. An example of non homogeneous equation is $dy/dx+y=3x$

A differential equation can be linear and homogeneous equation. An example of linear homogeneous equation is $dy/dx + = 0$ It can be linear non homogeneous.

This is called a linear non-homogeneous equation. An example of linear non homogeneous equation is $dy/dx + y = 3x$. All these types of differential equation can be of first order or second order or otherwise.

These are further categorized as first order homogeneous, first order linear, first order exact and variable separable equations. Second order equations are also further classified or non linear, homogeneous or non homogeneous differential equations.

CHAPTER TWO

2.1 FIRST ORDER REACTIONS

Let us consider a first reaction, let a be the initial concentration of the reactant A and X the concentration which has reacted at the time (in order words $\propto = x/a$ is the fraction of A which has reacted). Obviously the concentration present at time is a-x and we have

$dx/dt = k(a-x)$

To integrate this differential equation separate the variables

i.e. $\int dx/(a-x) = \int kdt$

$Ln\ a/(a-x) = kt$

which may be written as

$(a-x)ae^{-kt}$

If log a/(a-x) is plotted as a function of t gives a straight line graph of slope(-k). The units of the first order constant are S^{-1}

For example:- The liquid phase dissociation of dicyclopentadience has been studied longer and patton using gas chromatographic techniques. The techniques involved measured a quantity proportional to dc/dt rather than -dc/dt

Solution:-

Then, one can apply first order equation as dctdt = kc (rather than -dc/dt). The one of the reactant and the positive of the products.

$\int dc/c = \int kdt$

$Lnc = kt+c$

If $t = 0$

$c = lnc_o$

then, the equation becomes

$lnc = lnc_o + kt$

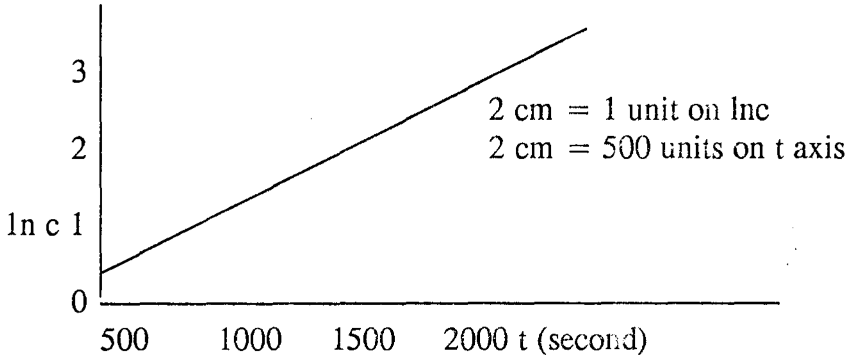
Where c and c_o are the equations that are proportional to the concentration. The value of k can be determined from the following data at 190°c

(a) separating the variables and integration have

C (c_o) t(second) Lnc

1.85	524	0.6125
2.04	620	0.7129
2.34	752	0.8502
2.70	876	0.9933
3.83	1188	1.3428
5.25	1452	1.6585

Then, one can plot graph of lnc against t a straight line which is linear is obtained as first order reaction satisfy.



22. SECOND ORDER REACTIONS

If we call a and b the initial concentration of the reactions A and B respectively in the following type of reaction.

A + B -> products

and x the concentration of A and B reacted at time, it is evident that $dx/dt = k(a-x)(b-x)$.........................(1)

(a) if, at the start, the reactants are of equal concentration (a = b), this equation becomes

$dx/dt = k(a-x)^2$

(b) $dx/dt = k(a-x)^2$ This expression is also obtained for a reaction of the type A+A -> products.

And X the concentration of A and B reacted at time t, it is evident that $dx/dt = k(a-x)(b-x)$.......................(1)

(a) if at the start, the reactants are of equal concentration (a=b), this equation becomes

$dx/dt = k(a-x)^2$

This expression is also obtained for a reaction of the type

$A+A \rightarrow$ Products

Separating the variables and integration have

$\int dx/(a-x)^2 \int kdt$

$1/(a-x) = k+c$ (where c is constant)

with the condition that $x = 0$ at $t = 0$ the constant become $1/a$ and the final expression is

$x/a(a-x) = kt$

b. if a and b are different (i.e. $b>a$), then separating the variables

$\int dx/(a-x)(b-x) = \int kdt$

By using the partial fraction we have

$1/b-a \ln(b-x)(a-x) = kt+c$

if $a-x = 0$ at $f = 0$ one have

$-1/(b-a)\ln b/a = c$

then, the final expression becomes $1/(b-a) \ln a(b-x)/b(a-x) = kt$

it is clear that if the reaction is really second order, then

(1) for the case $a = b$, if we plot $x/a(a-x)$ as a function of t a straight line will result which passes through the origin and slope ak i.e. if $a=b$

(2) if $a = b$, we plot $\log a(b-x)/b(a-x)$ as a function of t a straight line is also obtained. The units of the second order concentration are $mol^{-1} cm^3 \ S^{-1}$

2.3 THIRD ORDER REACTIONS

A third order reaction may be first order with respect to three reactants of A.B and C such that the rate of the reaction is then of the form $V = K.[A].[B].[C]$. it may also be of third order with respect to a single reactant when $V = K[A]^3$ i.e.

$V = dx/dt$ or first order with respect to another

i.e. $V = K[A].[B]^2$

of these three types of reactions, the last is the most frequent

The rate expression for the first of these corresponding to the reaction these are

$A+B+C \rightarrow$ products

This is easily to integrate if the initial concentration of the three reactants are equal (a=b=c)

and one have

$V= dx/dt = K.(a-x)^3$

The above equation is known as the case of third order reaction with respect to a single reactant. And if one integrate have

$\int dx/(a-x)^3 = \int kdt$

$1/2(a-x)^2 = kt+c$(where c is constant)

when $x = 0$ at $t = 0$ then, the constant is equal to

$1/2a^2 = c$ and the final equation becomes

$2kt = 1/(a-x)^2 - 1/a^2$

if t is plotted as function of $1/(a-x)^2$, straight line of slope 2k is obtained. The constant k is expressed in units of time^{-1} concentration^{-2} (i.e. $t^{-1}c^{-2}$)

Example:- For the reaction

$A+B+C \rightarrow$ products, with $C_{A,o} \neq C_{B,o} \neq C_{c,o}$,the differential rate equation is $dx/dt = -dc_A/dt$

$= kC_A C_B c_c$ ....(i)

and the integrated equation is

$$KT \quad \frac{Ln\,(C_A/C_{A,O}+\ln(C_B/C_{B,O})+(C_c/C_{c,O})}{(C_{A,O}-C_{B,O})(C_{c,O}-C_{A,,O})(C_{A,O}-C_{B,O})(C_{B,O}-C_{c,O})(C_{B,O}-C_{c,O})(C_{c,O}-C_{A,O})}$$

Where $C_{A,O}$ is a concentration of order A and C_A = concentration of A, for further reaction.

For the case where $C_{B,o} \neq C_{A,o} = C_{c,o}$ in equation (i) above, the reaction is 2A+B ->product(2 atoms combined in presence of another molecule) Where $C_{A,o} \neq C_{B,o} = C_{c,o}$,

The differential rate equation is

$$\frac{-dc_A}{dt} = KC_A 2C_B \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

and the integrated equation is $\frac{2}{(2C_{B,O}-C_{A,O})^2}\left[2\frac{(2C_{B,O}-C_{A,O})(C_{A,O}-C_A)}{C_{A,O}C_A}+\frac{LnC_{B,O}C_A}{C_{A,O}C_B}\right] = kt$

For the reaction $A+B \rightarrow$ Products, with $C_{A,O} \neq C_{B,O}$ Where equation (2) is valid, the integrated form is

$$\frac{1}{(C_{B,O}-C_{A,O})^2}\ \frac{(C_{B,O}-C_{A,O})(C_{A,O}-C_A)}{C_{A,O}C_A}+Ln\frac{C_{B,O}C_A}{C_{A,O}C_B} = kt\ldots\ldots\ldots(3)$$

For the case where $C_{A,O} = C_{B,O} = C_{c,O}$ for the equation (i) or $C_{A,O} = C_{B,O}$ or $C_{A,O} = 2C_{B,O}$ for equation (2) or for the reaction 3A-> products, the differential rate equation is $-dc/dt = kc_3 \ldots(4)$ which integrates to gives

$$\text{i.e } \int\frac{-dc}{C_3} = \int kdt$$

$$=> -{}^1/{}_2 LnC^2\ x\text{-}1 = kt+C \text{(where C is constant)}$$

$$=> {}^1/{}_2 \ln C^2 = kt+C \text{ if } t = 0 => C = 1/2LnC^2{}_0 \text{ the equation becomes}$$

$^1/_2\ lnC^2 = kt + 1/2lnC_o^2 => 1/2lnC^2 - 1/2lnC_o^2 = kt$

$=> {}^1/_2(C^2 - C_o^2) = kt$

or $^1/_2(1/C^2 - 1/C_o^2) = kt$

If one plots the graph of equation (1) or (2) or (4) against t a straight line is obtained which is linear and slope in each case equal to k

2.4 ZERO ORDER REACTIONS

These occur when the rate is entirely independent of the concentration of reacting substance.

i.e $V = k$ i.e $dx/dt = V = k$

$=> dx/dt = k$

Here n is zeroExample The decomposition of some gases, such as ammonia, on metal catalysts. For the overall reaction i.e A->products, the differential rate equation is

$Rd[A]/dt = k[A]_o$

$=> -A[A] = kdt$

integrating gives

$-[A] = kt + [A]$ where $[A]$ is constant, at $t = 0$

$=> -[A]_o = [A]$

Equation becomes

$-[A] = kt - [A]_o$ ....(7)

$[A] = -kt + [A]_o$

So, in the zero order case also a plot of concentration verses time a straight line graph of slope (-k) is obtained, the units zero order constant are mol cm $^{-3}$

2.5 HALF LIFE ORDER REACTION

Another important quantity is the reaction half life t1/2. It is the time at which the concentration of the reactant has fallen to half its value. Under these condition and taking into consideration that at t = t1/2 (in first order reaction is independent or the initial concentration at t = t1/2 then, $[A]t = 1/2[A]_o$ and this lead to $t1/2 = 1/k[A]_o$

If one plotted the graph against $1/[A]_o$. A straight line is obtained which is second order kinetics and the slope gives (-k)

Example:- The half life of a chemical reaction, t1/2 is defined by the condition [A]t = 1/2 at t = t1/2. For a zero order reaction in equation (7) gives

i.e $[A]t = 1/2[A]_o$..................................(8)

Put equation (8) into (7) and we have

i.e $1/2[A]_o = -kt+[A]_o$

$=> 2kt = 2[A]_o-[A]_o$

$2kt = [A]_o$

but t = t1/2

$=> t1/2 = 2[A]_o/2k$

TABLE (RATE EXPRESSIONS)

Let list the differential equation at order reaction in the table below

Order	Differential	Integral	t1/2 reaction half life
0	dx/dt = k	kt =x	
1	dx/dt= (a-x)	kt =k loga/(a-x)	t1/2=1/k
2	dx/dt = $k(a-x)^2$	kt =1/(a-x)-1/a	t1/2=1/ka
2	dx/dt = k(a-x)(b-x)	kt =k/(b-a)loga(b-x)/b(a-x)	
3	dx/dt = $k(a-x)^3$	kt $=1/2[1/(a-x)^2-1/a^2]$	
3	dx/dt $=k(a-x)^2(b-x)$	kt=1/(b-a)[x-k loga(b-x)/a(a-x)(b-a)	t1/2=$1/ka^2$

2.6 A REACTIONS OF SIMPLE ORDER (EQUATIONS OF FIRST ORDER AND FIRST DEGREE)

These equations only contain dy/dx and a function of x and y and are of the general form of equation

dy/dx+f(x,y)=o

The nature of above equation depends on function f(x,y) Example if f(x,y)is a function of x alone, the solution of the problem simply involves integration if dy/dx=f(x)

y=[f(x)dx+c(where c is arbitrary constant)

2.7 VARIABLES SEPARABLE

The equation of the form

$dx/dt=k(a-x)(b-x)$can be solve by separable variable as

$dx/(a-x)(b-x)=kdt$

Then, one can integrates both sides $\int dx/(a-x)(b-x)=\int kdt$

$1/a-b \ln (a-x)(b-x)=kt+c$(where c is constant), and assuming at $t=o,x=o$

$=> 1/a-b \ln(a/b) = c$

Then, the above equation becomes

$1/a-b \ln (a-x)/(b-x) = kt + 1/a-b \ln (a/b)$

$=> 1/a-b \ln(a-x)/(b-x)-1/a-b \ln(a/b) = kt$

$=> 1/a-b [(a-x)/(b-x)/a/b] = kt$

$=> 1/a-b \ln(a-x)b/(b-x)a = kt$

$=> 1/a-bin(a-x)/a(b-x) = kt$

Example:- $xcosy-e^{-x} secy\ dy/dx = 0$

Rearranging gives

$Sec^2 dy = xe^x dx$

$\int sec^2 ydy = \int xe^x$ but $sec^2 y = tany$

$tany = \int xe^x dx\ uv - \int vdu$

$=> tany = xe^x - \int e^x dx$

$tany = xe^x - e^x + c$

$=> tany = e^x (x-1)+c$

2.8 HOMOGENEOUS EQUATION

A function $f(x,y)$ is said to be homogeneous of degree n if $f(\lambda x,\lambda y) =\lambda nf(x,y)$

Example:- the function x^4-x^3y is homogeneous and of degree 4 since

$f(\lambda x, \lambda y) = (\lambda x)^4-(\lambda x)^3(\lambda y) = \lambda^4(x^4-x^3y) = \lambda^4f(x,y)$

Where as the function $x^4-x^3+y^2$ is not homogeneous i.e $f(\lambda x,\lambda y) =(\lambda x)^4-(\lambda x)^3 \neq \lambda nf(x,y)$

A homogeneous first order differential equation is of the form $A(x,y)dx+B(x,y)dy = 0$

where $A(x,y)$ and $B(x,y)$ are homogeneous functions of the same degree.

i.e $A(\lambda x,\lambda y) = \lambda n\ A(x,y)$ and $B(\lambda x,\lambda y) = \lambda nB(x,y)$

such equation can often be reduced to the variable separable type by the substitution

$y = vx$

Example $dy/dx =(9x^2+2xy+3y^2)/2x(x+y)$ is homogeneous of degree two

Applying the chain rule to y vx gives

$dy/dx = xdv/dx+v$ and $y/x = v$ and eliminating and dy/dx from equation (1)

i.e $xdv/dx+v = (9x^2+2xy+3y^2)/2x(x+y)$

$xdvdx+v =9+2v+3v^2/2(1+v)$

$=> xdv/dx = 9+v^2/2+2v$

which is now of the variable separable type. Separable of the variables gives

$\int dx/x = \int 2(1+v)dv/v^2+9$

$Lnx = ln(v^2+9)+2/3\ tan^{-1}v/3+c$

The general solution is obtained by substituting for v to give

$Lnx =ln\ (y^2/x^2+9)+2/3tan^{-1}y/3x+c$

2.9 EXACT DIFFERENTIAL EQUATIONS

The exact differential equations is of the form

$M(x,y)dx+N(x,y)dy=O$ is exact if

$\partial M(X,Y)/\partial Y=\partial N(X,Y)/\partial X$

The consequence of this is that some function

$Z=f(X,Y)$exists such that

$\partial Z/\partial x=M(x,y);\partial Z/\partial y=N(X,Y)$

If one have differential equation

$M(x,y)dx+N(x,y)dy=O$ and the left hand side is an exact differential dZ, then dZ is zero and f(x,y)is a constant. The solution of this equation is equivalent to the determination of the function f(x,y) often this can be done by inspection For example

$(4x^3y^3-2xy)dx+(3x^4y^2-x^2)dy=o$

Here $\partial Z/\partial x=4x^3y^3-2xy$, $\partial Z/\partial y=3x^4y^2x^2$ and one see of once that

$Z = x^4y^3-x^2y$

Thus, the solution to the equation is

$x^4y^3-x^2y=C$

One can proceed more formally as follows:-Given

$M(x,y)dx+N(x,y)dy=O$

We are looking for function $Z=f(x,y)$such that

$\partial Z/\partial x=M(x,y)$and $\partial Z/\partial y=N(X,Y)$

let us integrate with respect to x

$Z(X,Y) \int M(x,y)dx+\varnothing(x)$

Since Z is a function of two variables, the constant of integration will be a function of y

To determine $\varnothing(y)$, we now consider the y derivative of $ZN(x,y)=\varnothing Z/\varnothing y=\varnothing/\varnothing y$

$[\int M(x,y)dx+\varnothing(y)]$

This enables us to find $\varnothing(y)$ and hence the function Z

Example $(y^2e^{xy2}+4x^3)dx+(2xye^{xy2}-e^{xy2})dy=O$

$Z(x,y) = \int y^2e^{xy2}+4x^3)dx+\varnothing(y)$

$= e^{xy2}+x^4+\varnothing(y)$...............(2)

But $\partial Z/\partial Y$ must be equal to $2xye^{exy2}-3y^2$

From the equation (2) above

$\partial Z/\partial y = 2z/2y = 2xye^{xy2}$

and hence, $d\varnothing/dy$ must be equal to $-3y^2$and $\varnothing=-y^3$

Thus $Z(x,y)=e^{xy2}+x^4\ y^3$

and the general solution to the equation A above is

$=>e^{xy2}+x^4-y^3=C$

Differential equation occurring in practice are rarely exact but can often easily be transformed into exact equations by use of integrating functions

For example

$dy/y+[1/x-x/y]dx=O$

Here, is not exact, but multiplication by xy gives

$xdy+(y-x^2)dx=O$

Which is now exact and can be solved by inspection to give the general solution

i.e. $[xy-x^3]/3 = C$

2.10 LINEAR EQUATIONS

A particular important type of differential equation is the linear equation which has the general form.

$dy/dx+p(x)y=Q(X)$

The equation is of the form

$dx/dt+-kt$ for successive first order reaction.

To solve linear equation is to find an integrating factor $U(x)$ that will transform $dy+p(x)dx$ into exact differential. Thus, one require $U(x)dy+p(x)u(x)dx$.

To be an exact differential, there is some function

$Z=f(x,y)$ such that

$\varnothing Z/\varnothing x=p(x)$ and $\varnothing z/\varnothing y=u(x)$

Applying the criterion for an exact differential we get

$\varnothing u/\varnothing x(x) = \varnothing/\varnothing y\ [p(x)u(x)y]$

i.e. $\varnothing u/\varnothing x(x) = p(x)u(x)$

Hence, $1/U\varnothing u/\varnothing x = p(x)$

$\varnothing/\varnothing x \ln u(x) = p(x)$

$\ln u(x) = \int p(x)dx$ and $u(x) = e^{p(x)}dx$

then, the equation becomes

$e^{p(x)dx} dy/dx + p(x)y\ e^{p9x)dx} = Q(x)e^{p(x)dx}$

The left-hand side is the differential of $ye^{p(x)dx}$ and the equation becomes

$d/dx\ [ye^{p(x)dx}] = Q(x)e^{p(x)dx}$

We shall now apply this technique to the differential

equation for successive first order reaction consider the process

$A^{k1} \rightarrow B^{k2} \rightarrow C$ in which the concentration of A,B, and $C \rightarrow A^{K1} \rightarrow B^{k2} \rightarrow C$

at time t are a, b and c respectively, and rate constant for

the two reactions are k_1 and k_2.The rate of appearance of A is given by $da/dt = k^{1a}$

which has the solution

$a = a_o\ e^{-k,t}$

Where is the concentration of A at time t = O the rate of change of concentration of B is

given

$db/dt = k_{1a}\text{-}k_2b = k_1a_oe^{(k,t)}\text{-}k_2b$

$db/dt + k_2b = k_1a_oe^{-k,t}$

Multiplying by the integrating factor $e^{(sk_2dt)} = e^{k_2t}$ Gives $\rightarrow e^{(sk_2dt)} = e^{k_2t}$

$\rightarrow e^{k_2} + db/dt + k_2be^{k_2t} = k_1a_oe^{(k_2\text{-}k_1)t}$

Which can be rewriting as $\rightarrow d/dt(be^{k_2t}) = k_1a_oe^{(k_2\text{-}k_1)}t$

Therefore,

$\rightarrow be^{k_2t} = k_1a_oe^{(k_2\text{-}k_1)t} + C$

and applying the initial condition that t = O, b = O leads to the equation of the solution

$b = k_1\ a_o[e^{-k_1t}\text{-}e^{-k2t}]$

Example:-The equation

$(x-2)dy/dx=y+2(x-2)^3$

is linear as can be seen by rearranging it to give

$dy/dx=y/(x-2)+2(x-2)^2$

in this case the integrating factor is

$e\int -dx/(x-2) = 1/x-2$

and the equation becomes

$[1/x-2]dy/dx-y/(x-2)^2=2(x-2)$

i,e $d/dx[y/(x-2)=2(x-2)$

Therefore.

$y/(x-2)=(x-2)^2 + C$

$y=(x-2)^3 + c(x+2)$

2.11 RADIOACTIVE DISINTEGRATIONS

Among reaction of first order, particular mention must be made of those reactions for which the rate is always proportional to the remaining concentration of radioactive substance, with a constant proportionality h, independent of temperature. If Nt represents the number of radioactive atoms present at a time t, we have

$dNt/dt=hnt$

Then, if No is the initial number of atoms, can be written as the first order law

i.e. $Nt = Noe^{-nt}$

Where h is characteristics of the substance under study and is called the disintegration or decay constant

2.12 B COMPLEX REACTIONS (FIRST EQUATION OF HIGHER DEGREE)

These are of little importance in chemistry and we have the following

2.13 LINEAR SECOND ORDER DIFFERENTIAL EQUATIONS

These equations have the general form

$d^2y/dx^2+x)dy/dx + q(x)y=f(x)$

If $f(x)=o$, the equation is termed homogeneous, where as equation with $f(x)\neq 0$ are inhomogeneous. Here one shall be concerned only with the case in which p(x) and q(x)are constants, that is with linear equation and constant coefficients

Before consider the solution of second order equation let us look again of the first order case consider the equation

$dy/dx+xy=f(x)$............1

$\rightarrow dy/dx+xy=$.............2

That is, the inhomogeneous and homogeneous case

Equations are above has the solution

$y=e^{-ax\int f(x)}e^{axdx}+ce^{-ax}$

Whereas equation(2)above has the solution

$Y=ce^{-ax}$

Thus, the solution to the inhomogeneous equation consists of the general solution to the homogenous or reduced equation plus another term, which is a particular solution (the solution with $c=o$) to the inhomogeneous equation is the general function. This is also true for second order equation so one can write general solution =particular solution complementary function. Thus the solution of a linear second order inhomogeneous differential equation with constant coefficients involve two processes, the solution of the reduced equation and the determination of a particular integral

2.14 SOLUTION OF THE HOMOGENEOUS EQUATION

Consider the equation

$d^2 y/dx^2+ady/dx+by=o$

Let $D=d/dx$(differential operator

i.e. $D^2Y+aDy+by=o$

One can envisage factorising this by the methods of elementary algebra to give

$\rightarrow(D-K_1)(D-K_2)Y=0$

Remembering that D is an operator Expansion gives

$D^2y-(k_1+k_2)Dy+k_1k_2y=o$ and one see that k_1 and k_2 are roots of the auxiliary

equation $=>k_2+ak_1+b=o$

The general solution to the homogeneous equation $k_1\neq k_2$ i.e.

$=>y = c_1e^{k_1x}+c_2e^{k_2x}$

Where c_1 and c_2 are arbitary constant. This is a result that can be remembered easily

Example:- Find the general solution of D^2y-Dy-6y = o

solution

The Auxiliary equation is m^2-m-6 = o

(m+2)(m-3) = o

So, its roots are m = -2, m = 3. The general solution of the differential equation is

y = $c_1e^{-2x}+c_2e^{3x}$ (Where $c_1$and c_2 are arbitrary constants)

2.15 SOLUTION OF THE INHOMOGENEOUS EQUATION

The solution of this type of equation is more difficult and one still only consider a method applicable to fairly straight forward cases. More powerful method such as the D - operator method. The general solution of an equation of this type can be exposed as the sum of complementary function

$d^2y/dx^2+ady/dx+by = f(x)$

$2A-10Ax-5B+6Ax^2+6Bx+c = 4x^2$

Equating the coefficient of x^2 one have

6A = 2/3

Equating the coefficient of x, we have

-10A+6B = o

=>6B = 10*2/3

=>6B = 20/3

=>6B =20/18=10/9

Equating the constants term, one have

$2A-5B+6C = o$

$6C = 5B+2A$

$6C = 5*10/9+2*2/3$

$6c = 50/9+4/3$

$6c = 38/9$

$C = 19/27$ $y_p(x) = 2/3x^2+10/9x+19/27$

The general solution is $y(x)-y_c(x)+y_p(x)$

$y(x) = C_1e^{2x}+C_2e^{3x}+2/3x^2+10/9+19/27$

REACTIONS IN OPPOSITION

These types of reaction based on forward and backward reactions and one shall treats the following

2.16 THE TWO REACTION IN OPPOSITION ARE OF THE FIRST ORDER

The equilibrium is the form

The function f(x) is polynomial

For example. Find the general solution of $D^2y-5Dy+6y=4x^2$

Solution

One begin by finding the general solution of complementary equation

$D^2y-5Dy+6y = o$

The auxiliary equation for this homogeneous equation is

$m^2-5m+6 = o => (m-2)(m-3) = o$

The roots are $m = 2$ and $m = 3$. Thus, the general solution of $y_c(x)$ of the complementary equation is

$y_c(x) = C_1e^{2x}+C_2e^{3x}$

Where C_1 and C_2 are arbitrary constants

The technique is try the polynomial

Ax^2+Bx+C

and to determine coefficient A,B,C such that the polynomial

solution of the equation

Thus

$y_p = Ax^2+Bx+C$

$y^1_p = 2Ax+B$

$y''_p = 2A$

Then, substitute in to general equation have

$2A-5(2AX+B+6(AX^2Bx+c)=4x^2$

Now determine A,B and C by equating the right hand sides of equation

$$R \rightleftarrows P$$

Let a be the initial concentration of R, when the concentration of P is zero, x and x_e represen

the concentration of R at time t and at equilibrium (t=2) respectively

$dx/dt = K_1\rightarrow(a-x)-k_1\leftarrow x$

$e = k_1\rightarrow(a-x_e)-k_1\rightarrow x_e$

If one compare this with the expression

$dx/dt = k_1\rightarrow(a-x)$its order reaction

Obtained for a complete reaction one can conclude, as a treaty stated, that as a general rule this reaction can be mathematically treated as if it were complete the initial concentration a being replaced x_e and the rate constant by the sum

$(k_1\rightarrow+k_1\rightarrow)$. One can immediately obtained

$(\rightarrow k_1+\rightarrow k_1)t = \ln x_e/x_e-x$

Example:- Maturation of ∝-glucose, which in solution is partially transformed into B-glucose according to an equilibrium reaction. This cases a variation of the specific rotation [∝], of polarised light. The following data was obtained of 150°c

TIME	O	4	O
[∝]	110	74.6	52.6

Solution

Form this one can obtain $(\rightarrow k_1+\rightarrow k_1)$in min^{-1}, although the specific rotation of B- glucose is not given, it will be recalled that the difference from the initial value is proportional to the function of substance transformed

$x/x_e = (110-74.6)/(110-52.6) = o.616$

$(\rightarrow k_1+\rightarrow k_1)*4=\log x_e/x_e-x=\log 1/(1-x)/x_e$

Hence, $\rightarrow k_1 + \rightarrow k_1 = 1/4 \log 1/(1-0.616)\text{hour}^{-1}$

In min^{-1} this becomes

$\rightarrow k_1 + \rightarrow k_1 = 0.0017319 \text{ min}^{-1}$

Example 2 Given an equilibrium whose forward and backward reactions are first order, express the reaction half-life as a function of k and k_1 discuss

Solution :- Making use of the relationship previously demonstracted one can replace

$x = a/2$ for $t_{\frac{1}{2}} = t_{1/2}$

$k_1 + k_1 = 1/t_{1/2} \ln x_e/x_e{}^{-a/2} = 1/t_{1/2} \ln (1-a/2x_e$

x_e can be easily be found in terms of k

$x_e/a-x_e = k$

Hence $x_e = a.k/(k+1)$

and therefore,

$1-a/2x_e = k-1/2k$

hence

$=> {}^{\rightarrow}k_1 + {}^{\leftarrow}k_1 = 1/t_{1/2} \ln 2k/(k-1)$

Dividing both sides by $\rightarrow k_1$

i.e. $1+1/k = -1/\overset{\rightarrow}{k_1} t_{1/2} \ln 2k/(k-1)$

hence, $t_{1/2} = 1/k_1(1+k) \ln 2k(k-1)$

if $k<1$, $t_{1/2}$ has no meaning. To understand for this one need only examine the expression for x_e as a function of k

i.e. $(x_e = ak/k+1)$;

Under these conditions

$x_e > a/2$ and it is therefore, impossible to transform one-life of the initial reactant

2.17 THE TWO REACTION IN OPPOSITION ARE SECOND ORDER

The equilibrium is of the form

$$=> R_1 + R_2 \leftrightarrows P_1 + P_2$$

To simplify this, let assume that the initial concentration of R_1 and R_2 are equal to a, and that of P_1 and P_2 are zero

Consider $V = dx/dt$

One simply replace k by

$=> k_2.a(2x_e-a)/xe^2$,a by x_e and b by $ax_e/2x_e-a$

If this is done in the integrated equation are arrive at

$t = x_e/2k_2\ a(a-x_e)\ \ln x(a-2xe+ax^3)/a(x_e-x)$

Example;- How many days are required to transform one-life of the alcolol in the esterificatio of an equimolar,2/3 of the alcohol is transform and that is 64 days 1/4 has been transformed?

Solution

One will make use of the preeceding formula by letting

$x_e = 2a/3$

One will first apply it to the case of hand

t unknown, $x = a/2$, and then to know case

$t = 64$, $x = a/4$

t = constant. Ln $(2a^2-a^2)/36\ /(3a-a)/2$

=>64=constant. ln $(2a^2-a^2)/312*a(2/3a-a/4)$

Dividing the first equation by the second

t/64 = ln3/ln14 = log3/log14 = 3.35

Example 2 The equilibrium constant of the esterification reaction

$CHOOH+C_2HSOH\_\ H_2O\ +CH_3COOHS$

is H and both the forward and backward reactions obey, veri Hoff's low. A small quantity of acetic acid is dissolved in 50% by weight aqueous alcohol. Calculate k_2b knowing that after 159 minutes one quarter of the acid has reacted

Solution

Molecular weights of water = 18

Molecular weights of alcohol = 46

At equilibrium

$[Ester]_e[water]_e[Alcohol]_e = \overset{\rightarrow}{}k_2/\leftarrow k_2 = k = 4$

But in 50% aqueous alcohol

[water]/[Alcohol] = m/18*46/m = 2.5

Since this ratio is the one in the equilibrium expression one can obtain

$[Ester]_e/[Acid]_e = 4/2.5 = x_e/1-x_e$

From which $x_e = 0.61$

To calculate k_2b one will apply the formula

i.e $k_2\rightarrow b+k_2\leftarrow c = 1/t\ \ln x_ee/x_e-x$

taking the following into consideration

$k_{2\leftarrow} = k_{2\rightarrow}/k = k_{2\rightarrow}/4$

$\Rightarrow C = 2.26$

One deduce that

$k_{2\leftarrow c} = 2.5/4\ k_{2\leftarrow b}$ and

$k_{2\rightarrow b} + k_{2\leftarrow c} = 6.5/4 k_{2\rightarrow b}$

and conclude that

$6.5/4 k_{2\rightarrow b} = 1/150 * 2.3 + \log 0.61/(0.61-0.25)$

and $k_{2\rightarrow b} = 2.2*10^{-3} \mathrm{min}^{-1}$

CHAPTER THREE

3.1 QUANTUM MECHANICAL PROBLEM

The application of quantum mechanical principle to chemical problems has revolutionised the field to chemistry our understanding of chemical bonding, spectral phenomena, molecular reactivates and various other fundamental chemical problems rest heavily an our knowledge of the detailed behavious of electrons in atoms and molecules.

In this chapter one shall described in detail some of the basic principles, methods and result of quantum chemistry that lead to our understanding of electron behaviour

3.2 CLASSICAL MECHANICS

The way in which classical mechanics describes systems can be illustrated by two equations and these are

1. One equation express the total energy of a particle in terms of its kinetic energy + mu^2, where u is its speed at the potential energy v at the location at the particle.

eg $E = 1/2\ mu^2+v$, v and u are function of t

in terms of the linear momentum $p = mu$

i.e $E = p^2/2m+v$

This equation can be used in a number of ways. Example:-

Since $p = mdx/dt$ it is differential equation for x as function of t and its solution gives the position (and momentum) of the particle as function of time. A statement of both x(t) and p(t) is called the trajectory of the particle. The simplest example of this procedure is the case of a uniform, constant potential, so that v is indendependent of x and t. Then with v set equal to zero for simplicity the equation is

$E = p^2/2m$ or $(2E/m)^{1/2} = dx/dt$

The solution being

$x(t) = x(0)+(2E/m)/ht$

The constant energy E can be expressed in terms of the initial momentum p(0) and so the trajectory is $U(t) = x(0)+p(0)t/m$

$p(t) = p(0)$

Hence, knowing the initial and momentum, all later positions and momentum can be predicted

2. The second law of motion: i.e $p^1 = f => dt/dt = f$

Where p^1 dp/dt, the rate of change of momentum which is proportional to the acceleration.

i.e $p^1 = m(d^2x/dt^2)$ end F is the acting on the particle. It following that if we know the force acting every where and at all times, then solving this equation will also give the trajectory. This calculation is equivalent to the one based on E.

For example consider the case of a particle that is subject to a constant force F for a time τ, and it then allowed to travel freely. The Newton's equation becomes

$dp/dt = F$, a constant, for time between $t = 0$ and $t = \tau dp/dt = 0$ for times later than $t = \tau$ the first equation had the solution $p(t) = p(0)+Ft 0 \leq t \leq \tau$ and at the end of period the particle's momentum is $p(t) = p(0)+p\tau$

Example 2

The harmonic oscillation occurs when a particle experience a restoring force with a straight linearly proportional to the displacement, so that $F = -kx$, being the force constant, a strong spring has a large force constant. The negative sign in F signifies that the force is directed opposite to the displacement when x is positive (displacement to the right), the force negative (pushing towards the left) and vice versa.

Newton's equation is now $m(d^2x/dt^2) = -kx$ and a solution is

$x(t) = A\sin wt$, with $w = (k/m)^{1/2}$

The momentum is mx, and so $p(t) = mwA\cos wt$

i.e. $x(t) = wA\cos wt$ but $p = m'x$

$\Rightarrow p(t) = m'x = mwA\cos wt$

3.3 THE DIFFERENTIATION OF OPERATORS WITH RESPECT TO TIME

The concept of the derivative of a physical quantity with respect to time cannot be defined in quantum mechanics in the same way as in classical mechanics. For the definition derivative in classical mechanics involves the consideration of the, values of the quantity of two neighboring but distinct instant of time. In quantum mechanics, however, a quantity wh at same instant has a definite value does not in general have definite values at subsequent instants.

Hence, the idea of the derivative with respect to time must be differently defined in quantum mechanics. It is natural to defined the derivative of a quantity f as the quantity who mean value is equal to derivative with respect to time, of the mean value f. Thus, we have the definition f = f starting from this definition, it is easy to obtain an expression for the quantum mechanical operator f corresponding to the quantity f. i.e. f = f

$= d/dt\int\Psi^* f\Psi dq$

$=\int\Psi^*\delta f/\delta t\psi dq+i/h \int(H^*\psi^*)f\psi dq-i/h\psi^*f(H\psi)dq$

Since the operator H is hermitian, we have

$\int(H^*\psi^*)(f\psi)dq = \int\psi^*Hf\psi dq$

Thus, $f = \int\psi^*(\delta f/\delta t)+(i/hHf-i/hfH)\psi dq$

Since, on the other hand, one must have by the definition of mean values

i.e $f = \int\psi^*f\psi dq$

It is seen that the expression in parenthesis in the integral is the required operator f

i.e $f= \delta f/\delta t +i/h(Hf-fH)$

If the operator f is independent of time t reduces a part from a constant factor, to the commulator of the operator f and the Hamiltonian

A very important class of physical quantities is formed by those whole operators do not depend explicity on time and also compute with the Hamiltonian, so that f = 0, such quantities are said to be conserved

For those f = f = 0, that is f is constant. In other wards, the mean value of the quantity remains constant in time. One can also assert that, if is a given function of the operator f

3.4 THE SCHRODINGGER EQUATION

In 1926 Erwin schrodinger proposed an equation which, when solved, gives the wave function for any system. Position is as central to quantum mechanics as Newton's equations one to classical mechanics. Just as Newton's equation were an inspired postulate which, when solved give the trajectories of particles, so schrodinger's equation can be regarded as an inspired postulate which solved gives wave function. For a particles of mass m moving in one dimension with energy E the equation is

$-(h^2/2m)d^2\psi/dx^2 = E\psi$ and a solution is

$\psi = e^{ikx} = coskx + isinkx$ where $k = \sqrt{2mE/h^2}$

Coskx or Sinkx is a wave of wave lenght $\lambda = 2\pi/k$. This can be seen by comparing coskx th standard form of a harmonic wave, i.e. $\cos 2\pi x/\lambda$

The energy of the particle is entirely kinetic because $v = 0$ every where and so

$E = p^2/2m$

But since, the energy is related to by $E = k^2h^2/2m$ it follows that $p = kh$

Therefore, the linear momentum is related to the wave length of the $p = kh =$

$(2\pi/\lambda)(h/2\pi) = h/\lambda$

i.e. $p = 2\pi/\lambda^{*}h/2\pi = h/\lambda$

Which is the Broglies relation. If the particle is in a region where its potential energy is uniform but non zero, the Schrodinger equation is

$(-h^2/2m)d^2\psi/dx^2 = (E-V)\psi$

3.5 THE PARTICLE IN A ONE-DIMENSIONAL "BOX"

For one-dimensional system one have

$(-h^2/2m)d^2\psi/dx^2 + V\psi = E\psi$, $V = v(x)$, $\psi = \psi(x)$

or $d^2\psi/dx^2+(2m/h^2)(E-V)\psi = 0$

V is the potential energy of the particle

For example, for a free particle $v = 0$ (or some constant) and for a harmonics oscillator

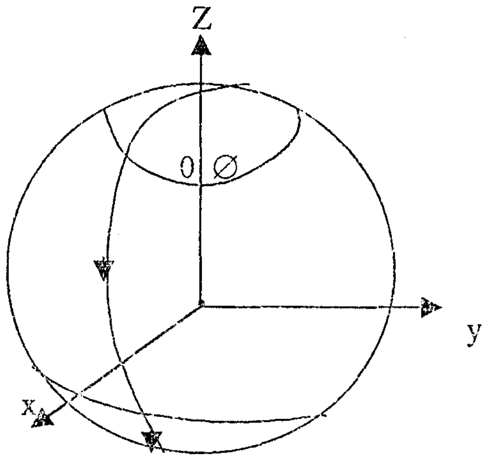
$V = 1/2kx^2$

For three-dimensional system

$(-h^2/2m)V^2\psi+V\psi = E\psi$, $V(x,y,z)$, $\psi = \psi(x,y,z)$ where $\nabla^2 = (\delta^2/\delta x^2)+(\delta^2/\delta y^2)+(\delta^2/\delta z^2)$.

In system with spherical symmetry z it is more appropriate to take ψ as a function of the spherical polar co-ordinates

see fig(1)



Then, we have

$\nabla^2 = (\delta^2/\delta r^2)+(2/r)(\delta/\delta r)\ (1/r^2)\Delta^2$

Where $\Delta^2 = (1/\sin^2\theta)(\delta^2/\delta\theta^2)+(1/\sin\theta)(\delta/\delta\theta\sin\theta(\delta/\delta\theta)(\delta/\delta\theta)$ in the general case,

the schrodinger equation is written as $H\psi = E\psi$

Where H is Hamiltonian operator for the system

$H = (h^2/2m)\nabla^2 + V$

When the system is time-dependently, use the time- dependent schrodinger equation is

$H\psi = i\hbar(\delta\psi/\delta t)$

But $E-V - h^2k^2/2m$

Now the relation $\lambda = 2\pi/k$ leads to

$\pi = h/(2m(E-V)/1/2)$

3.6 THE POTENTIAL FOR THREE DIMENSIONAL HARMONIC OSCILLATOR

$v = dx/dt = 1/2kx^2+1/2ky^2+1/2kz^2$ and the schrodinger equation for this problem is

$\delta^2\psi/\delta x^2+\delta^2\psi/\delta y^2+\delta^2\psi/\delta z^2 +8\pi^2/h^2M[E-1/2kx^2-1/2ky^2-1/2kz^2] = 0$ -----(1)

Where $\psi(x,y,z)$ is the wave function, m is the mass of the particle, h is plank's constant. E is the total energy and v is the potential energy.

The one using the separation of variables approach and write the wave function (x,y,z) in product form i.e $\psi(x,y,z) = x(x)y(y)z(z)$ and subsititute into equation (1) we have

$Y(y)Z(z)\delta^2/\delta x^2+X(x)Z(z)\delta^2 y/\delta y^2 + X(x)Y(y)\delta^2 Z/\delta z^2+8\Pi^2 m/h^2$

$[E-1/2kx^2+1/2ky^2+1/2kz^2]\ X(x)Y(y)Z(z) = 0$

If one introduce the separation constant Ex,Ey, Ez such that

$E=Ex+Ey+Ez$

One can separate equation (2) into three one-dimensional equations

i.e $1/X(x)d^2x(x)dx^2+8\pi^2m/h[Ex-1/2kx^2]=o$

$1/Y(y)d^2/dy^2+8\pi^2m/h^2[Ey-1/2ky^y]=o$

$1/Z(z)d^2Z(z)/dz^2+8\pi^2m/h^2[Ez-1/2kz^2]=o$

In this example one have carried out the separation in cartesian co-ordinates, but this may not necessarily always be the best co-ordinates system, it is better to the spherical polar co-ordinates in the case of the hydrogen atom, where the potential is of the form $1/\sqrt{(x^2+y^2+z^2)}$.

The schrodinger equation in polar co=ordinates for the hydrogen atom is

$1/r^2\propto r/\propto r[r^2\propto\Psi/\propto r]+1/r^2 \sin\theta$

$\sin\theta\propto/\propto\theta[\sin\theta\propto\Psi]+1/r^2\sin\theta^2\propto^2\Psi/\propto\theta^2+8\pi^2m/h^2\pi\ [E+e^2/4\pi\Sigma]\Psi=o$ ----A

Where e is the electric charge and Σo is the permutivity of free space. One write the wave function in produced form

i.e $\Psi(r,\theta,\varnothing)=R\ (r)\theta(\theta)\varnothing(\varnothing)$

and proceed as before to substitute this into the original equation (a) to give

$\theta(0)\ \varnothing(0)1/r^2[\delta r/\delta]+R(r)\varnothing(\varnothing)/r\ \sin\theta\delta\theta/\delta 0]+1/\varnothing\delta^2\varnothing/\delta\varnothing^2+r^2\sin^2\theta\ 8\pi/h^2\ U[E+e^2/4\pi\Sigma or]=0$

At this stage we can separate to give two equations

i.e. $1/\varnothing(\varnothing)d^2\varnothing/d\varnothing^2=-m^2$ and

$\sin^2\theta/R(r)\delta/\delta r[r^2\ \delta R/\delta r]\ +\sin\ \theta/\theta(0)\ \delta/\delta 0]+1/\Phi(\Phi)\delta^2\Phi/\delta\Phi^2\ +r^2\sin^2\theta 8\pi^2U/h^2$

$[E+e^2/4\pi\Sigma or]-m^2=0$

Rearrangement gives

i.e. $1/R(r)\delta/\delta r[r^2\ \frac{\delta R]}{\delta r}+\frac{1}{\theta(\theta)}\ \sin\ \frac{\theta\delta}{\delta\theta}\ [\sin\theta\ \frac{\delta\theta]}{\delta 0}+\frac{8}{h^2}\pi\frac{Ur^{22}}{}[E+\frac{4^2}{4\pi\Sigma_o r}]-\frac{M^2}{\sin^2\theta}=0$

Which can also be separated to give

$1/\theta(0)\ \sin d/d\theta[\sin\theta d\theta/d0]-M^2/\sin^2\theta=-E$

nd $1/R(r)\ d/dr\ [r^2 dR/dr] - B + 8\pi^2 Ur^2/h^2 [E + e^2/4\pi \Sigma_o r] = 0$

Thus, the separation of variables technique results in the resolution of the partial differential quation (A) in three dimensional in to the following ordinary differential equation

.e $d^2\Phi(\Phi)/d\Phi^2 = -m^2\Phi(\Phi)$

$$\frac{1}{\sin\theta}\frac{d}{d0}\left[\sin\theta \frac{d\theta}{d\theta}(\theta)\right] + B\theta(\theta) - \frac{m^2\theta(\theta)}{\sin^2\theta} = 0$$

$$\frac{1}{r^2}\frac{d}{dr}\left[r^2\frac{dR}{dr}(r) - B\frac{R(r)}{r^2} + \frac{8\pi^2 U}{h^2}\left[E + \frac{e^2}{4\pi\Sigma_o r}\right]R(v) = 0\right.$$

The first of these is a standard form and has the general solution

$\Phi(\Phi) = C_1 e^{im\Phi} + C_2 e^{-im\Phi}$

3.7 THE WAVE EQUATION

The vibration of a string, for example, is described by the wave equation

$V^2\delta^2 \psi \delta x^2 - \delta^2\psi/\delta t^2 = 0$ ....(1)

Where x is the position along the x-axis the time and Ψ is the displacement of the string perpendicular to the x-axis

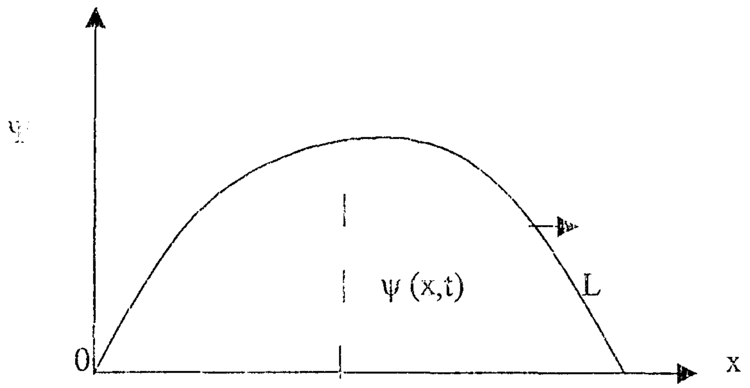


fig 2

Let consider a string of length L when it is unstreched and assume that it is fixed at the points x = 0 and x = L as shown fig (2) above

i.e. $\psi(0,T) = \psi(L,T) = 0$, for $T \geq 0$ (B)

The constant V is given by

$dx/dt = V = \sqrt{T}/M$

Where T is the tension and M is the mass per unit length we shall also have to specify the shape of the string when it is released at time $t = 0$

Let this be defined by a function f(x)

$\psi(u,0) = f(x)$, for $0 \leq x \leq L$

We also have to specify the value at $t = 0$ of the derivative of ψ with respect to t.

Let this be g(x)

i.e $\delta\psi/\delta t(x,t)g(x)$, for $0 \leq x \leq L$..................(1)

These are the boundaries condition which will enable us to give a specific solution for a particular set of initial condition

The technique of separation of variable assumes that we can write the solution U(x,t) as a product of two function of a single variable x(x) and T(t)

i.e $\psi(x,t) = X(x).T(t)$..........................(2)

and uses the assumption to reduce the partial differential equation to two ordinary differential equations, which hopefully, can be solved by standard techniques

Substituting equation (2) into equation (1) gives

$$V^2 T(t)\,\frac{\delta^2 X(x)}{\delta x^2} - X(x)\,\frac{\delta^2 T(t)}{\delta t^2}$$

That is

$$V^2 \frac{1}{X(x)}\,\frac{\delta^2 X(x)}{\delta x^2} - \frac{1}{T(t)}\,\frac{\delta^2 T(t)}{\delta t^2}$$

In this equation the left-hand side depends only on x and the right hand side only on t Since x and t are independent of each other, each side of this equation must be equal to a constant so we can write

$$\left.\begin{aligned} V^2 \frac{1}{X(x)}\,\frac{\delta^2 X(x)}{\delta x^2} &= -w^2 \\ V^2 \frac{1}{T(t)}\,\frac{\delta^2 T(t)}{\delta t^2} &= -w^2 \end{aligned}\right]\ldots\ldots\ldots\ldots(3)$$

Where $-w^2$ is the separation constant. Thus, we have two ordinary differential equations are

$$\left.\begin{aligned} V^2 \frac{1}{X(x)}\,\frac{d^2 X(x)}{dx^2} &= w^2 \\ V^2 \frac{1}{Tt}\,\frac{d^2 T(t)}{dt^2} &= -w^2 \end{aligned}\right]\ldots\ldots\ldots\ldots\ldots\ldots(4)$$

Which are both of the form of equation of simple harmonic motion which is

$d^2x/dt^2 = -w^2x$

We can therefore, write down their general solution as

$X(x) = A\cos(wx/v) + B\sin(wx/v)$

$T(t)\cos(wt) + D\sin(wt)$

Where A,B,C and D are arbitary constants whose values are to be determined from the boundary conditions the function $\psi(x,t)$ is then given by

$\psi(x,t) = (A\cos wx/v = B\sin wx/v)(C\cos wt+D\sin wt)$

The condition that $\psi(0,t) = 0$ gives

$0 = (A\cos\theta+B\sin\theta)(C\cos wt+D\sin wt)$

So, $A = 0$. Similary requiring that $(x,y) = 0$ gives

$0 = (B\sin wt/v)(C\cos wt+D\sin wt)$

since $B= 0$ would give the trivial solution $(x,y) = 0$, we require $\sin(wt/v)$ be zero and hence

$wt/v = n\pi$

Where $n = 1,2,3......$

Thus, we have

$$\psi(x,t)= \sin\left[\frac{n\pi x}{t}\right] [C_1 \cos wt+D_1 \sin wt]$$

Where $C_1 = BC, D_1 = BD$

Since n can be have an infinite number of values, there is an infinite number of solution

$$\psi_n(x,t) = \sin\left[\frac{n\pi x}{t}\right][C_n \cos wt+D_n \sin wt]$$

Which satisfy the boundary conditions of equation (b). Any linear combination of these functions is also C_n and D_n in such a way as to satisfy the boundary conditions of equation (D) and D when $t = 0$ we have

$\psi_n(x,0) = \Sigma C_r \sin(r\pi x/1)[C_r \cos\theta + D_r \sin\theta]= f(x)$

From equation C_r so in order to determine the coefficients C_r are require the fourier expansion of $f(x)$ in the interval

$0 \leq x \leq 1L$

Similarly the condition of equation D leads to the following expression for the value of the derivatives $\delta\psi/dt$ at $t = 0$

$$\text{i.e } \delta\psi/dt(x,t) = \sum_{r=1}^{\infty} (-C_r \sin wt + D_r \cos wt) w \sin[\pi rx]/lt = 0$$

$$= \sum_{r=1}^{\infty} D_r w \sin\left[\frac{\pi rx}{L}\right] = \frac{\pi v}{L} \sum_{r=1}^{\infty} r D_r \sin\left[\frac{\pi rx}{L}\right]$$

$$\text{i.e } g(x) = \frac{\pi v}{L} \sum_{r=1}^{\infty} r D_r \sin\left[\frac{\pi rx}{L}\right]$$

for the interval $0 \leq x \leq l$

But taking care to change the variable to allow for the interval being from 0 to l, gives the following values for the coefficient C_r and D_r

$$\text{i.e } C_r = Z/L \int_0^L f(x) \sin\left[\frac{\pi rx}{L}\right] dx$$

$$\Rightarrow D_r = \underline{2} \int_0^L g(x) \sin\left[\frac{\pi rx}{L}\right] dx$$

3.8 LEGENDRE'S DIFFERENTIAL EQUATION

Legendre function arise as solution of the differential equation of the form

$(1-x^2)y^{11} - 2xy^1 + n(n+1)y = 0$ ....(1)

The general solution of equation (1) in the case where $n = 0,1,2,3$................ is given by

$y = C_1 p_n(x) + C_2 Q_n(x)$

Where $P_n(x)$ are polynomials and $Q_n(x)$ are called legendre functions of the second kind

The Q_n are unbounded at x ±legendre polynomials are defined by

$$P_n(x) = \frac{(2n-1)(2n-3)}{n!}\ldots 1[x^n - \frac{n(n-1)}{2(2n-1)}xn^{2-1} + \frac{n(n-1)(n-2)(n-3)}{2.4(2n-1)(2n-3)}X^{n+4}$$

The legendre polynomials can also be expressed by Rodriques formula which is given by

$$P_n(x) = \frac{1}{2^n n!}\frac{d^n}{dx^n}(X^2-1)n \text{ for } n = 0,1,2,3,$$

The first legendre polynomials are as follow

$P_0(x) = 1$

$P_1(x) = x$

$$P_2(x) = \frac{1}{2}(3x^2-1)$$

$$P_3(x) = \frac{1}{2}(5x^2-3x)$$

$P_4(x) = {}^1/_8\,(35x^4-30x^2+3)$

$P_5(x) = {}^1/_8(63x^5-70x^3+15x)$

3.9 RECURRENCE FORMULA

$$P_{n+1}(x) = \frac{2n+1}{n+1} X P_n(x) - \frac{n}{n+1} P_{n-1}(x)$$

$P^1_{n+1}(x) - P^1_{n-1}(x) = (2n+2)P_n(x)$

3.10 ORTHOGONALITY OF LEGENDRE POLYNOMIALS

Ex. Prove that $\int^1_{-1} P_m(x)P_n(x)dx = 0$ if $m \neq n$

Solution

Since, $P_m(x)$, $P_n(x)$ satisfy legendre's equation

i.e $(1-x^2)\,p_m^{11} - 2xP_m^{1} + m(m+1)P_m = 0$........(1) also

$(1-x^2)\,p_n^{11} - 2xP_n^1 + n(n+1)P_n = 0$ ....(2)

Then, multiplying the equation (1) by P_n and equation (2) by P_m and substituting, we have

$$(1-x^2)[P_n{}_m^{11} - P_m{}_n^{11}] - 2x[P_nP_m^1P_mP_n^1] = [n(n+1)-m(m+1)]p_n p_m$$

$$(1-x^2)d/dx[P_nP_m^{11} - P_mP_n^{11}] - 2x[P_nP_m^1\ P_mP_n^1] = [n(n+1)-m(m+1)]\ P_mP_n$$

Thus, by integrating we have

$$[n(n+1)-m(m+1)]\int_{-1}^{1} P_m(x)P_n(x)\,dx = (1-x^2)[P_nP_m^1 - P_mP_n^1]\int_{-1}^{1}$$

Then, since $m\neq n \Rightarrow \int_{-1}^{1} P_m(x)P_n(x)dx = 0$

3.11 SERIES OF LEGENDRE POLYNOMIALS

If $f(x) = \sum_{k=o}^{\infty} A_k p_k(x)$, $-1\leq x\leq 1$, show that

$$A_k = \frac{2k+1}{2}\int_{-1}^{1} P_k(n)f(x)dx$$

Solution

Multiplying the given series by $P_n(x)$ and integrating from -1 to 1, we have

$$\int_{-1}^{1} p_{m}^{1}(x)f(x)dx = \sum_{k=o}^{\infty} A_k \int_{-1}^{1} P_m(x)\, p_n(x)dx = A_m \int_{-1}^{1} [P_m(x)]^2 dx = \frac{2A_m}{2m+1}$$

Then as required, $A_m = \frac{2m+1}{2}\int_{-1}^{1} P_m(x)f(x)dx$

3.12 HERMITES DIFFERENTIAL EQUATION

An importantant equation which arieses in problems of physics is called Hermite's differential equation, it is given by

$Y^{11}-2xy^{1}+2ny = 0$..................(2)

Where $n = 0,1,2,3$.............

The equation (2) has polynomial solutions called Hermites polynomials given by Rodrigues formula

i.e. $H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx^n}(e^{-x^2})$ for $n = 0,1,2,3$.......

The first few Hermite polynomial are

$H_o(x) = 1$ $\qquad$ $H_1(x) = 2x$

$H_2(x) = 4x^2-2$ $\qquad$ $H_3(x) = 8x^3-12x$

3.13 RECURRENCE FORMULA FOR HERMITE POLYNOMIALS

$H_n(x) = 2xH_n(x)-2nH_{n-1}(x)$

$H^{1}_{n}(x) = 2nH_{n-1}(x)$

3.14 ORTHOGONALITY OF HERMITE POLYNOMIALS

From first problem of legendre we have

$$\int_{-\infty}^{\infty} e^{-x2} H_m(x)H_n(x)\,dx = 0 \text{ i.e } m = n$$

So that the Hermite polynomials are mutually orthogonal with respect to the weight or density function e^{-x2}

In the case where m = n we can show as in problem of legendre and we have

$$\int_{-\infty}^{\infty} e^{-x2}H_{n2}(x)\,dx = 2^n n! \sqrt{\pi}$$

From this, we can normalize the Hermite polynomials so as to obtain an orthogonal set

3.15 SERIES OF HERMITE POLYNOMIAL

Using the orthogonality of the Hermite polynomial it is possible to expand a function in a series having the form $f(x) = A_o H_o(x)+A_1 H_1(x)+A_2 H_2(x)t....$

Where $A_n = \dfrac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{\infty} e^{x2}f(x)H_n(x)\,dx$

3.16 LAGURRE'S DIFFERENTIAL EQUATION

Another differential equation of importance in physics is laguerr's differential equation given by

$Xy^{11}+(1-x)y^1+NY = 0$

Where n = 0,1,2,3.........

This equation has polynomial solution called laguerre polynomials given by

$$L_n(x) = e^x \frac{d^n}{dx^n} (x^n e^{-x}) \text{ for } n = 0,1,2,3........$$

Which is also referred to as Rodrigues formula for the laguerre polynomials

$L_o(x) = 1$ $L_1(x) = x$ $L_2(x) = x^2-4x+2$ $L_3(x) = 6-18x+9x^2-x^3$

3.17 SOME IMPORTANT PROPERTIES OF LAGUERRE POLYNOMIALS

1. Generating function $$\frac{e^{-xf}/(1-t)}{1-6} = \sum_{n=o}^{\infty} \frac{L_n(x)\ t_n}{n!}$$

2. Recurrence formula

$$L_{n+1}(x) = (2n+1) - x) L_n(x) - n^2 L_{n-1}(x)$$

$$L^1_n(x) - nL^1_{-n}(x)+nL^1_{-n}(x) = 0$$

$$XL^1_{-n}(x) = nL_n(x) - n^2 l_{n -1}(x)$$

3. Orthogonality $$\int_o^{\infty} e^{-x} L_m(x) L_n(x)\, dx = 0 \text{ if } m=n$$

$$(nl)^2 \text{if } m=n$$

4. Series Expansions

If $f(x) = A_o L_o(x) + A_1 L_1(x) + A_2 L_2(x)\ t..........$

Then, $A_n = \frac{1}{(nl)^2} \int_o^{\infty} e^{-x} f(x)\, L_n(x)\, dx$

Example

Prove that the laguerre polynomials $L_n(x)$ are orthogonal in $(0,\delta\_)$ with respect to the weight function $e^{-(x)}$

Solution

From laguerr's differential equation we have for any two laguerre polynomials

$L_m(x)$

$L+(1-x)L^{1}_{m}+mL_m = 0$............(1)

$XL^{11}_{n}+(1-x)L^{1}_{n}+nL_n = 0$............(2)

Multiplying these equations (1) by L_n and (2) by L_m and then subtracting and we have

$X(L_nL^{11}_{m}-L_mL_n^{11})+(1-x)[L_nL^{1}_{m}-L_mL_n] = (n-m)L_mL_n$

or $d/dx(L_nL^{11}_{m}-L_mL_n^{11})+(1-x)/x[L_nL^{1}_{m}-L_mL_n] =(n-m)/xL_mL_n-L_mL_n^{11}]= (n-m)/x$ L_mL_n

Multiplying by the integrating factor

i.e. $(1-x)/xdx = e^{inx-x} = xe^{-x}$.

This can be written as

$$\frac{d}{dx}(xe^{-x}(L_nL^{1}_{m}-L_mL_n^{1}) = (n-m)e^{-x}L_mL_n$$

So that by integrating from 0 to ∞, we have $(n-m)\int_{0}^{\infty} e^{-x}L_m(x)\,L_n(x)\,dx = x\,e^{-x}(L_nL^{1}_{m}-L_mL_n)\int_{0}^{\infty}$

Thus if $m^{1}n$

$=> \int_{0}^{\infty} e^{-x}L_m(x)L_m(x)L_n(x)dx = 0$

Which prove the required result

Exampie (2) Expand x^3+x^2-3x+2 in a series of languerre polynomials i.e. $\sum_{k=o}^{\infty} = 0\ A_kL_k(x)$

Solution

$x^3+x^2-3x^2+2 = A_o L_o(x)\ A_1 L_1(x) + A_2 L_2(x) + A_3 L_3(x) + \ldots\ldots$

Then, we need to applying the formula

$L_n(x) = e^x \frac{d^n}{dx^2}(x^n e^{-x})$ for $n = 0,1,2,3\ldots\ldots$

Therefore, $L_o(x) = L_1(x) = 1-x$

$L_2(x) = e^x \frac{d^2}{dx^2}\ (x^2e^{-x}) = 2-4x+x^2$

$L_3(x) = e^x \frac{d^3}{dx^3}(x^3e^{-x}) = 6-18x+9x^2-x^3$

Then, we have

$A_0 L_0(x)\ A_1 L_1(x)+A_2 L_2(x)+A_3 L_3(x) = x^3+x^2-3x+2$

$A_0 + A_1(1-x)+A_2(2-4x+x^2)+A_3(6-18x+9x^2-x^3)$

$(A_0 + A_1 + 2A_2 + 6A_3) - (A_1 + 4A_2 + 18A_3)x + (2A_2 + 9A_3)x^2 - A_3 x^3$

Then, equating like powers of x on both sides we have

$A_0 + A_1 + 2A_2 + 6A_3 = 2$ ……………………………………………(1)

$A_1 + 4A_2 + 18A_3 =$ ……………………………………………………(2)

$A_2 + 9A_3 = 1$ ……………………………………………………………(3)

$A_3 = 1$ ……………………………………………………………………(4)

Solving these, and we have

$A_0 = 7,\ A_1 = -19,\ A_2 = 10,\ A_3 = -1$

Then, the require expression is

$x^3 + x^2 - 3x + 2 = 7L_0(x) - 19L_1(x) + 10L_2(x) - L_3(x)$

CHAPTER FOUR

4.1 PROGRAM DEVELOPMENT/IMPLENTATION

PROGRAMMING LANGUAGE

Before looking into programming language in the computer, itself?

Computer can be defined as an electronic device which is used to input data (raw informatic processed the in-puted data, store the data in the man memory and give it out as output for fut managerial and administrative uses.

The programming language refers to the computer understands or converts to its mach code needed for the solution of a particular problem: The language of the computer have un one changes and development since the first set of computer programmes were written in bi based machine language.

The current used high level languages are Basic, Cobol, Fortran, Pascal etc. the com used high level language is basic. It is an acronym for, Beginners All symbolic instruction c The programming language is widely used because of its advantage in both commercial scientific application. It can also be converted into its various versions (GW Basic, Q B Turbo Basic), This language is capable of running the IBM and compatible computer systems.

4.2 CHIOCE OF PROGRAMMING LANGUAGE

The program at hand is academically in nature therefore we require a language, which is to write by non-programmers.

The problem to be solved is technical and so it requires proper planning and development good program to meet up the requirement.

Because of the above requirement Basic has been chosen as the most suitable language fo this project. Specifically, Q Basic is the program I used for this project work. Basic can be use for both commercial and scientific application. Basic also has some flexible features such a screen design to create user friendly screen, directly output to printer for the production of har copies. Basic is usually used and it is usually installed by most computer hardware manufacture without having to buy the software.

4.3 PROGRAMME INSTALATION AND OPERATION.

The installation of the program into the computer is quite easy.

This was done by creating a batch file solely for installation purposes.

The steps for installing the program are as follows:

1). Make sure your system is switched on and has booted successfully.

2). At the system prompt (i.e. C:/.>) change the derive to the diskette derive i.e. typing A: or B: at the prompt.

3). At the new prompt type STARTUP

4). The files to instalied are displayed

5) Answer the un-screen questions like strict any key to continue

6) You will also be required to supply the password to be used by the installation.

7) When you are true with the set up menu control will be taken back to the batch file in order perform the carrying of all files in the system diskette to the hard disk and latter returning you the system prompt.

4.4 STARTING THE PROGRAM

This refers to getting the program to use in order to solve the problem encountered when running the program.

1) At the system prompt (i.e. C:\>) or change the drive to the diskette drive (if you want to work on the diskette i.e. A: or B:)

2) Type file name at the prompt, and you are taken to the introductory part of the program. If usually shows the name of the software and other necessary information relating to the use of the program. After the introduction, down arrow keys or depressing the first letter of the intended menu can be using to select the option for the operation you want to perform. This will actually allow you to highlight the menu options but their selection is completed by repressing the enter key.

Program to solve reactions, kinetic and Quantum mechanical problems

```
10 Screen 9:Cls
20 Line (1,1)-(630,300), 4,B
30 Line (3,3)-(627,297), 4, B
40 Locate 4,30: Print "A Computer Programme for solving Reaction Kinetic "
50 Locate 6,35 : Print " And "
60 Locate 8,25 : Print "Quantum Mechanical Problems"
70 Locate 12,32 : Print "By"
80 Locate 12,27 : Print "Mohammed Abdullahi"
90 Locate 14,29 : Print "PGD/MCS/98/99/770"
```

```
100 Locate 20,24 : Print “Strike any key to continue “:A$=input$(1): Cls

110 Cls

120 Line (1,1)-(620,300), 4, B

130 Line (3,3)-(627,297), 4, B

140 Locate 3,5 : Print “Menu”

150 Locate 6,20 : Print “(1) Equation of Reactions”

160 Locate 8,20 : Print “(2) Add more value of t (N/Y)?”

170 Locate 10,20 : Print “(3) Exit”

180 Locate 20,40 : Print “ input select your choice”;ch

190 if ch = 1 then go to 240

200 if ch = 2 then go to 240

210  if ch = 3 then go to 230

211  220 if ch>1 or ch <> 2 or ch <> 3 then go to 110

230 Cls: Beep : Print “Program terminated” : End

240 Rem on ch

250 Cls

260 Print “dy/dt = kt”

270 input “Enter value of t”;t

280 input “Enter value of k” ;k

290 Ans = k*t

300 Print “dy/dt = “;Ans
```

```
310 Locate 25,10 : input “Goto the next page (Y/N)” ;R$

320 if R$= “y” then go to 110 Else : Cls : Print “Program terminated”

330 End
```

CHAPTER FIVE

5.1 FINDINGS SUMMARY AND RECOMMENDATION

It could be the major points to be used for any irrespectively students who want to be copy of this project, because it can help then in studies or researching their differential equation in related to chemistry.

The investigation of a reaction to determine the rate law and value of the rate constant, often at several temperatures, ideally, the first step is to identify all the products, and to investigate whether transient intermediates and side reactions are involved. The isolation method may then be used to examine the role of each component in turn, and to determine the order with respect to each one. The order with respect to each substance can be gulged form the method of initial slopes or the dependence of the half life of the concentration and then the order confirmed, and k determined by a plot of the appropriate function of the concentration against time using one of integrated laws expression such as equation (T) or equation (M). However, since all the laws considered so far disregarded the possibility that the reverse reaction is important, more of them is reliable when the reaction is close to equilibrium. Therefore, all plots can be expected to acquire some curative for times, so long that the reactions involving the products become important. In the case of more intricate rate laws (such as those we encounter later) the concentrations of reactants, intermediates and products are computed numerically and the rate constant are varied until the experimental data are produced.

Associated with any particle is a wave function having wave length relented to particle momentum by h = $\sqrt{2m(E-V)}$. The wave function ψ for time-independent states are eigen functions of Schrodinger equation can be constructed from the classical wave equation. The wave function for particle in a varying potential oscillation most rapidly. Find the condition that must be satisfied by α and β in order that $\psi(x) = A\sin\alpha x + B\cos\beta x$ satisfy.

CONCLUSION

This project has shown the basic definition of differential equations, and comput programme for solving reaction kinetics and quantum mechanical problems, wide explained and field work in kinetics mostly a straight lines (k constants) is obtained wh plotted on the graph. The structure manifests themselves in quantum properties.

The extend of congregation is a useful measure of bond length and is direc contributory to the total energy of the system.

RECOMMENDATIONS

Quantum mechanical prediction must approach classical prediction in the limits of large E, or large mass, or very high Quantum number value motion of a particle on a ring has Quantum mechanical solutions very similar or to those for free particle motion in one dimension. The basic steps were

1. Determine the a symbolic behaviour of the schrodinger equation and function. This produces a guess in factor exp(-$y^{2/2}$) times function of y, f(x).
2. Obtain a differential equation for the next of the wave function, f(y)
3. Represent f(y) as a power series in y, and find a recursion relation for the coefficien in the series. The symmetries of the wave, function are linked to the symmetries o the series. The schrodinger equation for an electron moving in the field of a fixed nucleus is almost identical with equation obtained from separation of variable i reduced mass co-ordinates in the moving, nucleus case. The bound state energies fo time independent states of the hydrogen like ion depend on the quantum number n (positive integer) and vary as $-1/n^2$. ψ describes a state as completely as possible an must meet certain mathematical requirements (single value etc) $\psi^*\psi$ is the densit distribution for the system for any observable these is an operator (hermitic) which i constructed from the classical expression according to a simple recipe if th Hamiltonian operator for a system is time independent, stationary eigen functio exist, and the time dependent exponential does not effect the measurable properties o a system in this state and is almost always completely ignored in any tim

independent problem. Any operation that leaves H unchanged also commutes with H. Recognise the polynomials are as being Hermite, Legendre and laguere polynomials and utilize some of the known properties of these functions to establish orthogonality and normalization constants for the wave function.

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