Project Report on

Transition probabilities in quantum dot with laser pulse using Runga Kutta method

Submitted For Phd Course Work

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Contents

Abstract

Here forth order Runga Kutta method is formulated with its physical interpretation. Further this method is extended to solve the n coupled equation. A program in FORTRAN to solve coupled equation using Runga Kutta Methods is shown. As the application of this numerical method, I have considered the laser pulse interaction with parabolic quantum dot. Time dependent Schrodinger equation is used to solve this combination and getting some coupled equation in the form transition probabilities, which are solved here using the FORTRAN programming and Runge kutta methods.

Introduction

The impressive progress in the fabrication of low-dimensional semiconductor structures during the last two decades has made it possible to reduce the effective device dimension from three-dimensional bulk materials, to quasi-two dimensional quantum well systems, to quasi-one dimensional quantum wires, and even to quasi-zero dimensional quantum dots. The modified electronic and optical properties of these quantum-confined structures, which are controllable to a certain degree through the flexibility in the structure design, have attracted considerable attention, and have made them very promising candidates for possible device applications in semiconductor lasers, microelectronics, non-linear optics, and many other fields. Quantum dots are small conductive regions in a semiconductor, containing a variable number of charge carriers (from one to a thousand), that occupy well-defined, discrete quantum states, for which they are often referred to as artificial atoms. There are several existing devices utilizing quantum effects in solids, such as **semiconductor resonant tunneling diodes** (based on quantum mechanical confinement), **superconducting Josephson junction circuits** (based on macroscopic phase coherence**), metallic single electron transistors** (based on quantization of charge), **molecular electronic devices** (based on the inter-dot coupling in a double quantum dot structure. In this report, i am going to focus on quantum dot which may be called as artificial atom [1].When a semiconductor sturucture is confined in all direction, their density of states becomes discrete like atoms as shown in fig 1.

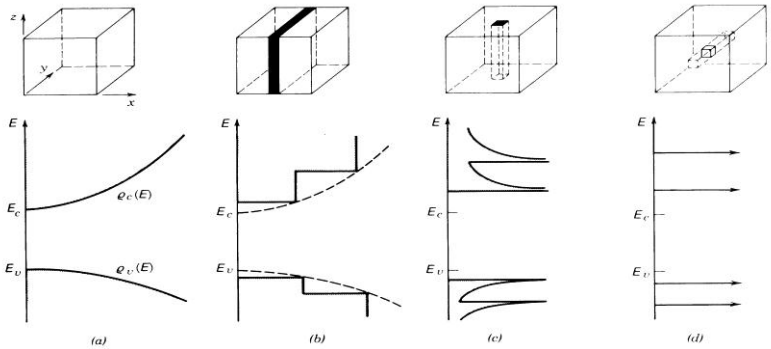


Fig 1. *Comparison of the quantization of density of states: (a) bulk, (b) quantum well, (c) quantum wire, (d) quantum dot. The conduction and valence bands split into overlapping subbands, that get successively narrower as the electron motion is restricted in more dimensions.*

The peculiar quantum behavior of electrons in quantum dots is under investigation in many laboratories around the world. The tunable size, shape and electron number, as well as the enhanced electron correlation and magnetic field effects, makes quantum dots excellent objects for studying fascinating many-electron quantum physics in a controlled way. I am here to study the pulsed laser effects on quantum dot to find the optical transitions.

A laser can be described as an optical source that emits a coherent beam of photons at an exact wavelength or frequencies. With the recent progress in ultrafast optics, it is now possible to

shape ultrashort laser signals with almost arbitrary temporal shapes. These shaped signals are generated from laser pulses through manipulation of the spectral phases and amplitudes of the frequency components of these pulses. With the ability to shape such pulses with high fidelity, excitations should not be limited to pulse pairs or simple pulse sequences, and it is natural to ask, then, what degree of control can be achieved by exciting quantum dot by such complex-shaped pulses. Coherent control strategies by tailoring ultrashort laser pulses are tremendously successful to manipulate the physical and chemical processes and properties. So it is very interesting to investigate theoretically the effects of ultrafast laser pulses on energy levels of quantum dot.

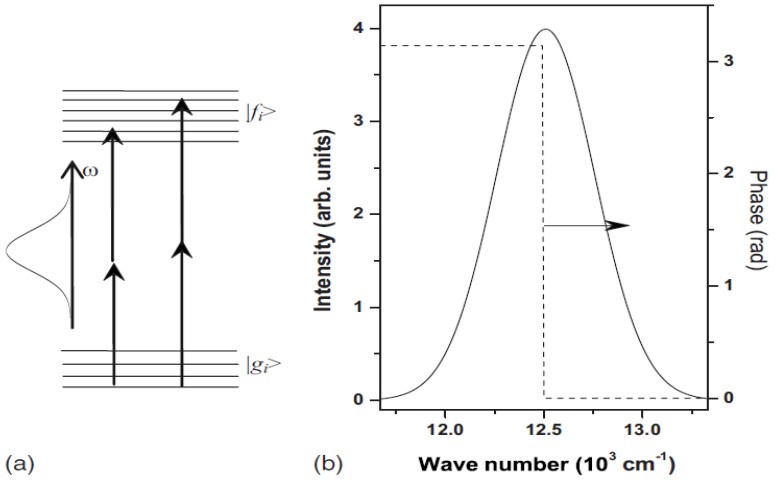


FIG. 2. (a) The schematic energy-level diagram of two-photon transitions in two-level system, the population is initially in the ground state. (b) The schematic diagram of a spectral phase step applied on the femtosecond laser spectrum.

To solve this fruitful combination for finding the probability evolution, at first interaction Hamiltonian is formulated and then time-dependent Schrödinger equation is solved by taking the expansion of wave function. Here we have got coupled time dependent differential equation. These equations can be sloved by many numerical techniques like density matrix approach, floquet theory etc, but here, we are using Runga Kutta method for findings the solutions. So at first Runga Kutta is discussed, and after that it is mentioned that how we can solve coupled equation using runga kutta method. Program of solution of various coupled equation in FORTRAN is also shown. After finding the solutions the results for optical transition probabilities are shown for quantum dot in the results section.

Runga Kutta Methods

The Runge–Kutta methods are an important family of implicit and explicit iterative methods for the approximation of solutions of ordinary differential equations. Runge-Kutta methods are single-step methods, however, with multiple stages per step. They are motivated by the dependence of the Taylor methods [2]. These new methods are stable and easy to program, therefore these are general-purpose initial value problem solvers. Runge-Kutta methods are

among the most popular ODE solvers. They were first studied by Carle Runge and Martin Kutta around 1900. Modern developments are mostly due to John Butcher in the 1960s.The Runge-Kutta 2nd order method is as follows:

For equation, $\frac{dy}{dx} = f(x, y),\ \ y(0) = y_0$

with intial condition, then solution is written as

$$y_{i+1} = y_i + \left(\frac{1}{2}k_1 + \frac{1}{2}k_2\right)h$$

where

$$k_1 = f(x_i, y_i)$$
$$k_2 = f(x_i + h, y_i + k_1 h)$$

Only first order ordinary differential equations can be solved by using the Runge-Kutta 2nd order method. In next sections, it is shown that how Runge-Kutta methods are used to solve higher order ordinary differential equations or coupled (simultaneous) differential equations.

Runge-Kutta 4th order method.

Runge-Kutta 4^{th} order method is a numerical technique used to solve ordinary differential equation of the form

$$\frac{dy}{dx} = f(x, y), y(0) = y_0$$

So only first order ordinary differential equations can be solved by using the Runge-Kutta 4^{th} order method. 4^{th} order means that in this method at every point four times the functions is used The Runge-Kutta 4^{th} order method is based on the following

$$y_{i+1} = y_i + (a_1 k_1 + a_2 k_2 + a_3 k_3 + a_4 k_4)h \qquad (1)$$

where knowing the value of $y = y_i$ at x_i, we can find the value of $y = y_{i+1}$ at x_{i+1}, and

$$h = x_{i+1} - x_i$$

Equation (1) is equated to the first five terms of Taylor series

$$y_{i+1} = y_i + \frac{dy}{dx}\Big|_{x_i, y_i}(x_{i+1} - x_i) + \frac{1}{2!}\frac{d^2y}{dx^2}\Big|_{x_i, y_i}(x_{i+1} - x_i)^2 + \frac{1}{3!}\frac{d^3y}{dx^3}\Big|_{x_i, y_i}(x_{i+1} - x_i)^3 + \frac{1}{4!}\frac{d^4y}{dx^4}\Big|_{x_i, y_i}(x_{i+1} - x_i)^4 \qquad (2)$$

Knowing that $\frac{dy}{dx} = f(x, y)$ and $x_{i+1} - x_i = h$

$$y_{i+1} = y_i + f(x_i, y_i)h + \frac{1}{2!}f'(x_i, y_i)h^2 + \frac{1}{3!}f''(x_i, y_i)h^3 + \frac{1}{4!}f'''(x_i, y_i)h^4 \qquad (3)$$

Based on solution of above equation peculiar results are:

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)h \quad (4)$$

$$k_1 = f(x_i, y_i) \quad (5a)$$

$$k_2 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1 h\right) \quad (5b)$$

$$k_3 = f\left(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2 h\right) \quad (5c)$$

$$k_4 = f(x_i + h, y_i + k_3 h) \quad (5d)$$

Physical interpretation: since we are using this function four times at every single point for going near to the original curve, this gives more accurate results as comparable to others methods. This is shown in Fig 3

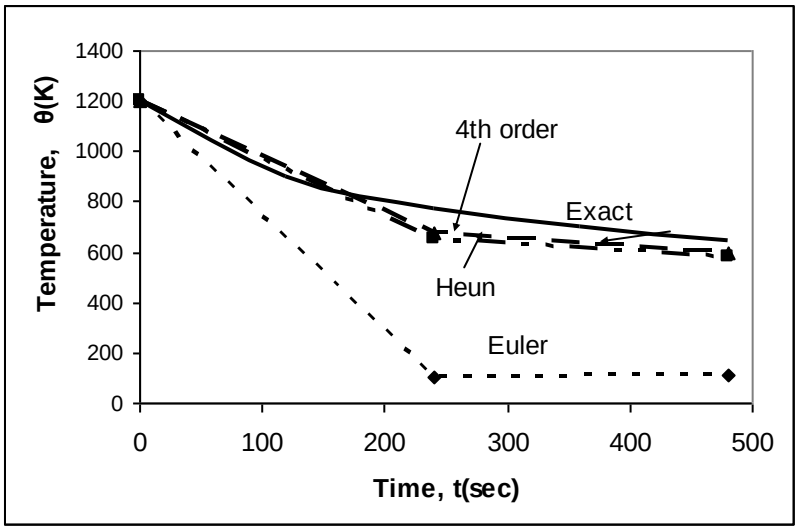


Fig 3 : Comparison of accuracy

Up to now we are able to solve first order differential equation accurately, but questions arises how we can solve many coupled equation and 2nd order equation. To solve this question we extend forth order solutions to two differential equations,

$$\frac{dy}{dx} = f(x, y, z) \quad \text{and} \quad \frac{dz}{dx} = g(x, y, z) \quad \text{with intitial conditions at } x = 0, y = y_0, z = z_0$$

Then the values of y_i and z_i are obtained as follows:

$$y_{i+1} = y_i + \frac{1}{6}\left(k_1^i + 2k_2^i + 2k_3^i + k_4^i\right)h \quad (6)$$

and $$z_{i+1} = z_i + \frac{1}{6}\left(l_1^i + 2l_2^i + 2l_3^i + l_4^i\right)h \qquad (7)$$

where

$$k_1^i = f\left(x_i, y_i, z_i\right)$$
$$l_1^i = g\left(x_i, y_i, z_i\right)$$
$$k_2^i = f\left(x_i + \frac{h}{2}, y_i + \frac{k_1^i}{2}, z_i + \frac{l_1^i}{2}\right)$$
$$l_2^i = g\left(x_i + \frac{h}{2}, y_i + \frac{k_1^i}{2}, z_i + \frac{l_1^i}{2}\right)$$
$$k_3^i = f\left(x_i + \frac{h}{2}, y_i + \frac{k_2^i}{2}, z_i + \frac{l_2^i}{2}\right) \qquad (8)$$
$$l_3^i = g\left(x_i + \frac{h}{2}, y_i + \frac{k_2^i}{2}, z_i + \frac{l_2^i}{2}\right)$$
$$k_4^i = f\left(x_i + h, y_i + k_3^i, z_i + l_3^i\right)$$
$$l_4^i = g\left(x_i + h, y_i + k_3^i, z_i + l_3^i\right)$$

In the same way we can formulate the solution of n equation , consider n equations are :

$$\frac{dx}{dt} = f_1\left(x, y, z, ..., t\right),$$
$$\frac{dy}{dt} = f_2\left(x, y, z, ..., t\right),$$
$$\frac{dz}{dt} = f_3\left(x, y, z, ..., t\right) \qquad (9)$$
$$.....$$
$$.....$$

with intial some intial conditions at $t = t_0, x = x_0, y = y_0, z = z_0.....$, then the solution of above equation can be written as

$$x_{i+1} = x_i + \frac{1}{6}\left(k_1^i + 2k_2^i + 2k_3^i + k_4^i\right)h$$
$$y_{i+1} = y_i + \frac{1}{6}\left(l_1^i + 2l_2^i + 2l_3^i + l_4^i\right)h$$
$$z_{i+1} = z_i + \frac{1}{6}\left(m_1^i + 2m_2^i + 2m_3^i + m_4^i\right)h \qquad (10)$$
$$.....$$
$$.....$$

Where

$$k_1^i = f_1\left(x_i, y_i, z_i, \ldots\ldots\ldots, t\right)$$
$$l_1^i = f_2\left(x_i, y_i, z_i, \ldots\ldots\ldots t\right)$$
$$m_1^i = f_3\left(x_i, y_i, z_i, \ldots\ldots\ldots t\right)$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$

$$k_2^i = f_1\left(x_i + \frac{k_1^i}{2}, y_i + \frac{l_1^i}{2}, z_i + \frac{m_1^i}{2}, \ldots\ldots\ldots, t_i + \frac{h}{2}\right)$$
$$l_2^i = f_2\left(x_i + \frac{k_1^i}{2}, y_i + \frac{l_1^i}{2}, z_i + \frac{m_1^i}{2}, \ldots\ldots\ldots, t_i + \frac{h}{2}\right)$$
$$m_2^i = f_3\left(x_i + \frac{k_1^i}{2}, y_i + \frac{l_1^i}{2}, z_i + \frac{m_1^i}{2}, \ldots\ldots\ldots, t_i + \frac{h}{2}\right) \qquad (11)$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$

$$k_3^i = f_1\left(x_i + \frac{k_2^i}{2}, y_i + \frac{l_2^i}{2}, z_i + \frac{m_2^i}{2}, \ldots\ldots\ldots, t_i + \frac{h}{2}\right)$$
$$l_3^i = f_2\left(x_i + \frac{k_2^i}{2}, y_i + \frac{l_2^i}{2}, z_i + \frac{m_2^i}{2}, \ldots\ldots\ldots, t_i + \frac{h}{2}\right)$$
$$m_3^i = f_3\left(x_i + \frac{k_2^i}{2}, y_i + \frac{l_2^i}{2}, z_i + \frac{m_2^i}{2}, \ldots\ldots\ldots, t_i + \frac{h}{2}\right)$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$

$$k_4^i = f_1\left(x_i + k_3^i, y_i + l_3^i, z_i + m_3^i, \ldots\ldots\ldots, t_i + h\right)$$
$$l_4^i = f_2\left(x_i + k_3^i, y_i + l_3^i, z_i + m_3^i, \ldots\ldots\ldots, t_i + h\right)$$
$$m_4^i = f_3\left(x_i + k_3^i, y_i + l_3^i, z_i + m_3^i, \ldots\ldots\ldots, t_i + h\right)$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$
$$\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots$$

Hence we can solve n coupled equation (10) as from the above numerical procedure. Now we are going to formulate the above numerical methods in terms of the FORTRAN program.

That is

```
SUBROUTINE RUNGE(ITYPE,N,NSTEPS,H,X,Y,XOUT,YOUT)

 PARAMETER(MEQ=N)
```

```
      REAL Y(MEQ)
      REAL Y0(MEQ)
      REAL K0(MEQ)
      REAL K1(MEQ)
      REAL K2(MEQ)
      REAL K3(MEQ)

      DO 40 J=0,NSTEPS
      CALL FUNC(K0,Y,X)
      DO 42 I=1,N
      Y0(I)=Y(I)
42    Y(I)=Y0(I)+K0(I)*0.5*H
      X=X+H*0.5
      CALL FUNC(K1,Y,X)
      DO 43 I=1,N
43    Y(I)=Y0(I)+K1(I)*0.5*H
      CALL FUNC(K2,Y,X)
      DO 44 I=1,N
44    Y(I)=Y0(I)+K2(I)*H
      X=X+0.5*H
      CALL FUNC(K3,Y,X)
      DO 45 I=1,N
45    Y(I)=Y0(I)+(K0(I)+2.0*(K1(I)+K2(I))+K3(I))/6.0*H
      C1=Y(1)**2+Y(2)**2
      C2=Y(3)**2+Y(4)**2
      ct=C1+C2
      WRITE(6,100) X,C1,C2,ct

 100  format (6f15.10)
40    CONTINUE
      RETURN
      END
```

So now we are able to solve n coupled equation using runga kutta method. Where the coupled equation arises? In the next section we will solve this question.

Laser pulse effect on Quantum dot

In this section we find the effect of laser pulse on the quantum dot. For this at first we will find the eigenergies ang eigenfunction of parabolic quatum dot and the take the laser pulse interaction as a perturbation and solve this combination using schrodinger wave equation by taking the epansions of wave function. We will get the coupled equation and these are solved by runga kutta methods for the transition probabilities. Here we are considering the only two lowest levels for conveniences.

Eig*en* energies and Eigen wavefunction of Quantum dot:

For our purpose, we are considering GaAs parabolic quantum dot with potential

$$V(r) = \frac{1}{2} m^* \omega_o^2 (x^2 + y^2) \tag{12}$$

Where m^* is the effective mass of electron in conduction band and ($\hbar\omega_0$) is the confinement potential strength corresponds to size of quantum dot. When this is placed in vertical magnetic fields [**B** = (0, 0, B)] in symmetric gauge vector potential $\mathbf{A} = \mathbf{B}(-y, x, 0)/2$, then the single electron in effective mass Hamiltonian without considering the spin is [1]

$$\mathrm{H}_0(\mathbf{r}) = \frac{1}{2m^*}(\mathbf{p} + e\mathbf{A})^2 + \frac{1}{2}m^*\omega_0^2(x^2 + y^2) \tag{13}$$

Eigen function of above Hamiltonian will be Fock-Darwin states $\Psi_{nl}(\mathbf{r}) = \frac{1}{\sqrt{2\pi}}R_{nl}(r)e^{il\phi}$, with

$$R_{nl}(r) = \frac{\sqrt{2}}{a}\sqrt{\frac{n!}{(n+|l|)!}}\exp\left(-\frac{r^2}{2a^2}\right)\times\left(\frac{r^2}{a^2}\right)^{|l|/2} L_n^{|l|}\left(\frac{r^2}{a^2}\right) \tag{14}$$

where $a = \left(\frac{\hbar}{m^*\Omega}\right)^{1/2}$, and $\Omega^2 = \omega_0^2 + \frac{\omega_c^2}{4}$, with $\omega_c = \frac{eB}{m^*}$ (cyclotron frequency). Eigen energies are as, $E_{nl} = (2n + |l| + 1)\hbar\Omega - \frac{\hbar}{2}l\omega_c$ (15) , where $n = 0,1,2,\ldots$, and $l = 0, \pm1, \pm2,\ldots$.

Interaction of Laser Pulse

Now laser pulse is applied on quantum dot. Laser pulse may be form of any shape like Gaussian, rectangular etc. in laser pluse electric field vary with time that can be written as

$$\vec{E}(t) = \hat{e}f(t)F_0 Cos(\omega t) \tag{16}$$

Where $\hat{e}$ is the unit polarization vector, F_0 is the maximal electric amplitude, And for pulse width τ , $f(t)$ is defined as

$f(t) = 1$, for $0 < t < \tau$

$= 0$, otherwise (17)

So, here in presence of laser pulse, total Hamiltonian can be written in to two parts one is time independent same as H_0 and other is time dependent part arises due to interaction with pulse laser fields as:

$$\mathrm{H}\ (\mathbf{r},t) = \mathrm{H}_0(\mathbf{r}) + \mathrm{H}_{\mathrm{int}}(\mathbf{r},t) \tag{18}$$

Where $\mathrm{H}_{\mathrm{int}}(\mathbf{r},t) = -e\vec{E}(t).\vec{r} = -\mu(r)\,f(t)F_0 Cos(\omega t)$ (19)

Where $\mu(r)$ is the QD dipole moment operator.

To solve this dynamical problem, we need to solve time – dependent schrodinger equation using the Hamiltonian of equation (18). So, the time evolution of the system wave function is determined by the

$$i\frac{\partial}{\partial t}\Psi_m(\mathbf{r},t) = \mathrm{H}\ (\mathbf{r},t)\Psi_m(\mathbf{r},t) \tag{20}$$

$\Psi_m(\mathbf{r},t)$ is the system wave function, 'm' denotes particular state having quantum number 'n,l', this wavefunction can be expended in terms of eigenfunction of Hamiltonian $\mathrm{H}_0(\mathbf{r})$ as

$$\Psi(\mathbf{r},t) = \sum_k C_k(t)\psi_k(\mathbf{r})e^{-\frac{i}{\hbar}\omega_k t} \tag{21}$$

Here 'k' denotes for the quantum number 'n,l' of the quantum dot. Using the expansion of the wave function $\Psi(\mathbf{r},t)$ and orthogonally of the Eigen states in (14), a set of coupled equation is obtained as

$$i\frac{\partial}{\partial t}c_b(t) = \sum_k \langle\psi_b|\mathrm{H}_{\mathrm{int}}|\psi_k\rangle c_k(t)e^{i\omega_{bk}t} \tag{22}$$

Where

$\omega_{bk} = \dfrac{E_b - E_k}{\hbar}$ is the bohr angular frequency, using equation (19), Eq.(22) becomes

$$i\frac{\partial}{\partial t}c_b(t) = \sum_k \mu_{bk}c_k(t)e^{i\omega_{bk}t}\,f(t)F_0 Cos(\omega t) \tag{23}$$

Here $\mu_{bk} = \langle\psi_b|\mathrm{H}_{\mathrm{int}}|\psi_k\rangle = \langle\psi_b|er|\psi_k\rangle$, are the dipole matrix element.

Equation (23) is the set of coupled equations, which are solved by Runga Kutta method as follows

Fortran program for Transition Probabilities

```
            IMPLICIT REAL (a-h,o-z)
            Dimension y(4),
            open (6,file='abc2')
            open (7,file='abc1')
            t=0.0
            y(1)=1.0
            y(2)=0.0
            y(3)=0.0
            y(4)=0.0
c-----------------------------------
            BE=1.0d0
c------ step size of Runge Kutta method H = dt = 0.1
            dt=0.1
c-------------------------
            nstep=8000
            t=0.0
            call RUNGE (4,nstep,dt,t,y)
            stop
            end

      FUNCTION pulse( ITYPE,E0,t,TP,TAU,OMEGA)
      GO TO (1,2,3,4) ITYPE
c-----------------------E(t)=E0
  1    pul=E0
      GO TO 5
c-----------------------E(t)=E0*e^[ {-(t-TP)**2}/2*TAU ]* Cos(omega* t)
  2    ENVELOP=EXP(-((t-TP)**2.0D0)/2*TAU)
      pul=E0*ENVELOP
      GO TO 5
c----------------------E(t)= E0* Gaussian
  3    ENVELOP=EXP(-(t**2.0D0)/2*TAU)
      pul=E0*ENVELOP
      GO TO 5
 4    IF (t.LE.TP) THEN
      ENVELOP=1.0d0
      ELSE
      ENVELOP=0.0d0
      ENDIF
      pul=E0*ENVELOP
      GO TO 5
  5    pulse=pul
      RETURN
            END

            subroutine FUNC(dy,y,t)
            dimension y(4),dy(4)
c------ Coupled Equations -------
c------- dy/dx = dy(1)=X* Y*z= t*Y(1)*Y(2)
c------  dz/dx = dy(2)=X*Y/z = t* Y(1)/Y(2)
c  **        dy(1)=y(1)*y(2)*t
c  **        dy(2)=y(1)*t/y(2)
c-----------------------------------------------
c           dy(1)=(y(2)-1.)*y(1)    !Eberly
c           dy(2)=-y(1)*y(2)       !Eberly Book
            E0=5.0d-1
            E1=0.0d0
            E2=2.0d0
            TP=5.0d0
            TAU=2.0d0
```

```
c       OMEGA=E2-E1
        OMEGA=(E2-E1)*0.9
c       hi1=pulse(1,E0,t,TP,TAU,OMEGA)
c       hi1=1.0d1
c       hi2=DCV(0,0,0,0,1.0d0,1.0d0)  !B=1.0d0; A_0=1.0d-2
c       hi=hi1*hi2
        hi=2.5d0
        funs1=funsi(t,E2,E1,OMEGA)
        func1=funcs(t,E2,E1,OMEGA)
        funs2=funsi2(t,E2,E1,OMEGA)
        func2=funcs2(t,E2,E1,OMEGA)
        dy(1)=(-y(3)*funs1+y(4)*func1)*hi
        dy(2)=-(y(3)*func1+y(4)*funs1)*hi
        dy(3)=(-y(1)*funs2+y(2)*func2)*hi
        dy(4)=-(y(1)*func2+y(2)*funs2)*hi
        write(7,101) t, hi1
 101    format(2f15.9)
        return
        end

        function funsi(t,E2,E1,omega)
        funsi=sin((E2-E1-omega)*t)
        return
        end

        function funcs(t,E2,E1,omega)
        funcs= cos((E2-E1-omega)*t)
        return
        end


        function funsi2(t,E2,E1,omega)
        funsi2= sin((-E2+E1+omega)*t)
        return
        end

        function funcs2(t,E2,E1,omega)
        funcs2= cos((-E2+E1+omega)*t)
        return
        end
        SUBROUTINE RUNGE(ITYPE,N,NSTEPS,H,X,Y,XOUT,YOUT)

        PARAMETER(MEQ=4)

        REAL Y(MEQ)
        REAL YOUT(MEQ)
        REAL Y0(MEQ)
        REAL K0(MEQ)
        REAL K1(MEQ)
        REAL K2(MEQ)
        REAL K3(MEQ)
        DO 40 J=0,NSTEPS
        SUM=0.0
        DO I=1,50
        NORM=Y(I)*Y(I)+Y(I+50)*Y(I+50)
        SUM=SUM+NORM
        END DO
        CALL FUNC(K0,Y,X)
        DO 42 I=1,N
        Y0(I)=Y(I)
 42     Y(I)=Y0(I)+K0(I)*0.5*H
        X=X+H*0.5
        CALL FUNC(K1,Y,X)
        DO 43 I=1,N
 43     Y(I)=Y0(I)+K1(I)*0.5*H
        CALL FUNC(K2,Y,X)
        DO 44 I=1,N
 44     Y(I)=Y0(I)+K2(I)*H
```

```
      X=X+0.5*H
      CALL FUNC(K3,Y,X)
      DO 45 I=1,N
45    Y(I)=Y0(I)+(K0(I)+2.0*(K1(I)+K2(I))+K3(I))/6.0*H
      C1=Y(1)**2+Y(2)**2
      C2=Y(3)**2+Y(4)**2
      ct=C1+C2
      WRITE(6,100) X,C1,C2,ct
100   format (6f15.10)
40    CONTINUE
      RETURN
      END


c--------This function will calculate the dipole matrix elements for SAME BAND (conduction-conduction) transitions.
      FUNCTION DCC(N,L,NP,LP,BE)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C     OPEN (6,FILE='test')
c     AC=SQRT(27.2D3/0.67D0)  !IN ATOMIC UNIT.. AC=sqrt[(hbar^2)/(m^* omega)]
c     AC=1.0d0
      AC1=(0.067d1/27.2d0)*sqrt((5.0d-3)**2 + (BE/(2.5d5*2.0d0*0.067d0))**2)
   AC=SQRT(1.00/AC1)
c     N=1
c     L=1
c     NP=0
c     LP=2
      SUM1=0.
      DO 05 IH=0,N
      DO 05 IK=0,NP
      COEF=(-1)**(IH+IK)
      L1=IABS(L)
      LP1=IABS(LP)
      GAM1=(L1+LP1+1)/2
      GAM2=IH+IK+1
      GAM3=GAM1+GAM2
      CALL LGAMA(1,GAM3,GAMA)   !GAMA((L+LP+1)/2 +IH+IK+1)
      CNL=C2(N,L,IH)
      CNLP=C2(NP,LP,IK)
      XX=1.0d0/(IFACL(IH)*IFACL(IK))
      SUM1=COEF*GAMA*CNL*CNLP*XX+SUM1
05    CONTINUE
      TERM1=C1(N,L,NP,LP)*AC/SQRT(2.0d0)
      DCC=TERM1*SUM1
C     WRITE(6,*)"SUM1,TERM1, DIOPLE", SUM1,TERM1, DIPOLE
      RETURN
      END



C======= THIS FUNCTION CALCULATES ^(N+|L|)C_(N-IH)
C-------
      FUNCTION C2(N,L,IH)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C     N=2
C     L=2
C     IH=1
      L1=IABS(L)
       AUM=FLOAT(IFACL(N+L1))
      NN=IABS(N-IH)
      DENO=FLOAT(IFACL(NN)*IFACL(L1+IH))
c     DENO=FLOAT(IFACL(N-IH)*IFACL(L1+IH))
      C2=AUM/DENO
C     WRITE(6,*)"NUM,DENO,C2", NUM,DENO, C2
      RETURN
      END


C=====================================================================
```

```
c----------This function will calculate {[(n!)*(np!)]/[(n+l)! *(np+lp)!]}^(1/2)* del_{l,lp}
C=====================================================================
C---------- (N & L) AND  (NP & LP) ARE THE PRINCIPLE AND ANGULAR QUANTUM NUMBERS OF THE TWO STATES in different
BANDS.
      FUNCTION CV1(N,L,NP,LP)
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      NUM=IFACL(N)*IFACL(NP)
            L1=IABS(L)
            LP1=IABS(LP)
      DENO=IFACL(N+L1)*IFACL(NP+LP1) !(N+L)! * (NP+LP)!
      IF (L.EQ.LP) THEN
      CV1=SQRT(NUM/DENO)
      ELSE
      CV1=0                !THE if STATEMENT GIVES THE DELTA FUNCTION.
      ENDIF
            RETURN
      END
C-----------------------------------


c----------This function will calculate {[(n!)*(np!)]/[(n+l)! *(np+lp)!]}^(1/2) *del_{l,lp+-1}
c (N & L) AND  (NP & LP) ARE THE PRINCIPLE AND ANGULAR QUANTUM NUMBERS OF THE TWO STATES in the same band...
            FUNCTION C1(N,L,NP,LP)
            IMPLICIT DOUBLE PRECISION (A-H,O-Z)
            NUM=IFACL(N)*IFACL(NP)
            L1=IABS(L)
            LP1=IABS(LP)
            DENO=IFACL(N+L1)*IFACL(NP+LP1) !(N+L)! * (NP+LP)!
            IF (L.EQ.(LP+1)) THEN
            C1=SQRT(NUM/DENO)
            ELSE IF (L.EQ.(LP-1)) THEN
            C1=SQRT(NUM/DENO)
            ELSE
            C1=0                !THE if STATEMENT GIVES THE DELTA FUNCTION.
            ENDIF
            RETURN
            END
C-----------------------------------
c----------THIS FUNCTION CALCULATES THE FACTORIAL OF NN..
      FUNCTION IFACL(NN)
      INTEGER NN,NN1,IFACL
      IFACL=1
      DO 11 NN1=1,NN
      IFACL=IFACL*NN1

 11    CONTINUE
      RETURN
      END

c---------------------------------

      SUBROUTINE GAMMA(X,GA)
C
C     ==================================================
C     Purpose: Compute the gamma function â(x)
C     Input :  x  --- Argument of â(x)
C                 ( x is not equal to 0,-1,-2,úúú )
C     Output:  GA --- â(x)
C     ==================================================
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      DIMENSION G(26)
      PI=3.141592653589793D0
      IF (X.EQ.INT(X)) THEN
        IF (X.GT.0.0D0) THEN
          GA=1.0D0
```

```
        M1=X-1
        DO 10 K=2,M1
10          GA=GA*K
      ELSE
        GA=1.0D+300
      ENDIF
    ELSE
      IF (DABS(X).GT.1.0D0) THEN
        Z=DABS(X)
        M=INT(Z)
        R=1.0D0
        DO 15 K=1,M
15          R=R*(Z-K)
        Z=Z-M
      ELSE
        Z=X
      ENDIF
      DATA G/1.0D0,0.5772156649015329D0,
     &       -0.6558780715202538D0, -0.420026350340952D-1,
     &       0.1665386113822915D0,-.421977345555443D-1,
     &       -.96219715278770D-2, .72189432466630D-2,
     &       -.11651675918591D-2, -.2152416741149D-3,
     &       .1280502823882D-3, -.201348547807D-4,
     &       -.12504934821D-5, .11330272320D-5,
     &       -.2056338417D-6, .61160950D-8,
     &       .50020075D-8, -.11812746D-8,
     &       .1043427D-9, .77823D-11,
     &       -.36968D-11, .51D-12,
     &       -.206D-13, -.54D-14, .14D-14, .1D-15/
      GR=G(26)
      DO 20 K=25,1,-1
20      GR=GR*Z+G(K)
      GA=1.0D0/(GR*Z)
      IF (DABS(X).GT.1.0D0) THEN
        GA=GA*R
        IF (X.LT.0.0D0) GA=-PI/(X*GA*DSIN(PI*X))
      ENDIF
    ENDIF
    RETURN
    END
```

Results and Discussion

Using the above numerical technique, coupled equations are solved, and we get the transition probabilities of electron between the energy levels of quantum dot causing by laser pulse, here we are using three different types of laser pulses. So we are getting three different transition probabilities between the first two levels.

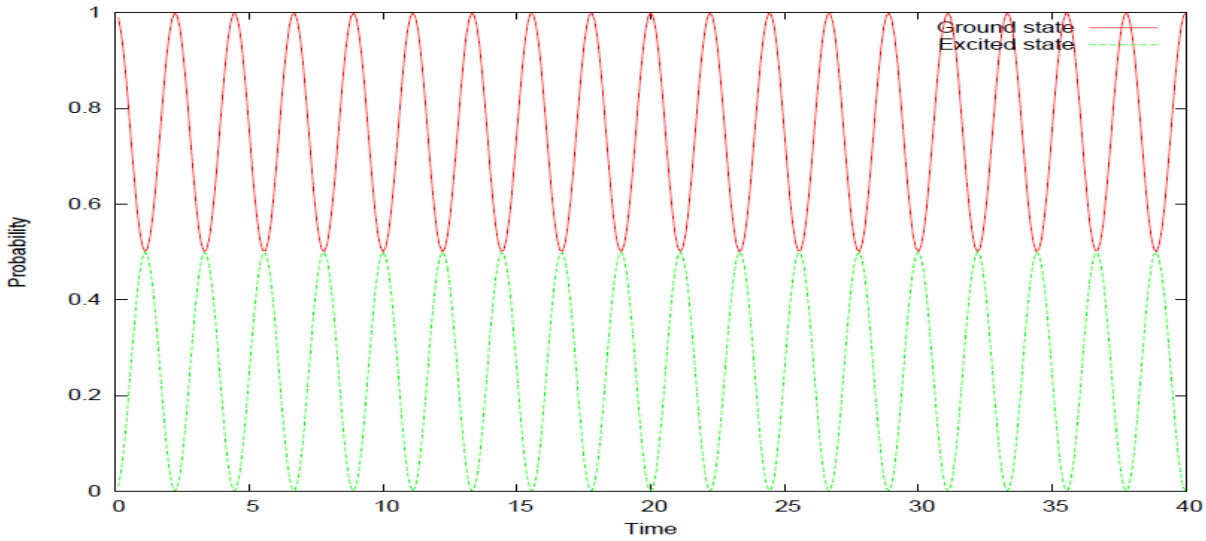


Fig 4 : transitition probabitlity between two lowest level are shown for the constant value of laser pulse electric field magnitude. These oscilation are known as rabi oscilations.

(1) for laser pulse with constant electric fields, the transition probabilities are shown in Fig4, on x axis the time scale is represented in seconds and on y axis the transition probability is shown. The upper curve showing the ground state probability and lower state showing first level transistion probability.

(2) for Gausisan laser pluse (as shown in Fig5) the transition probabilities are shown in fig6

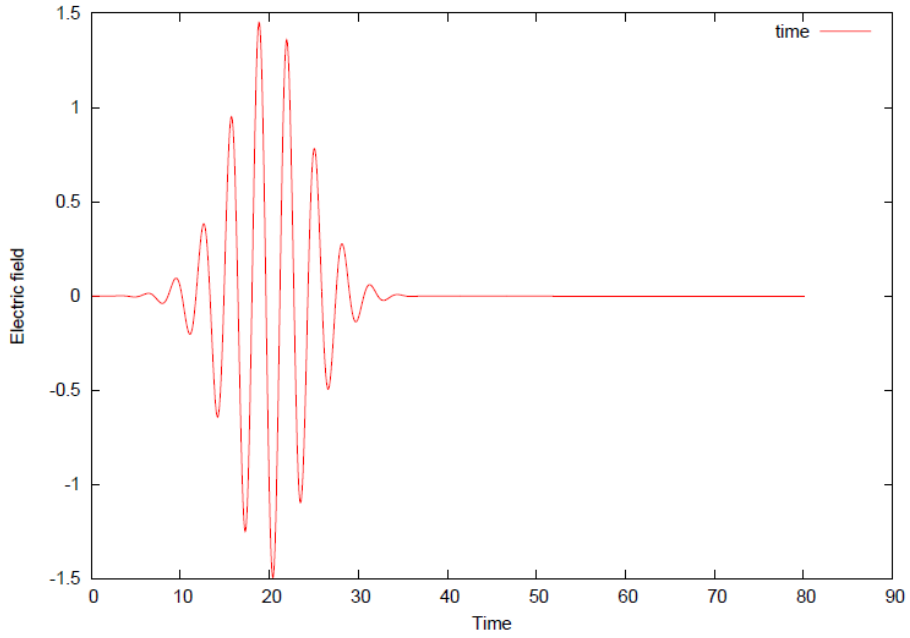


Fig5: Gaussian pulse shape

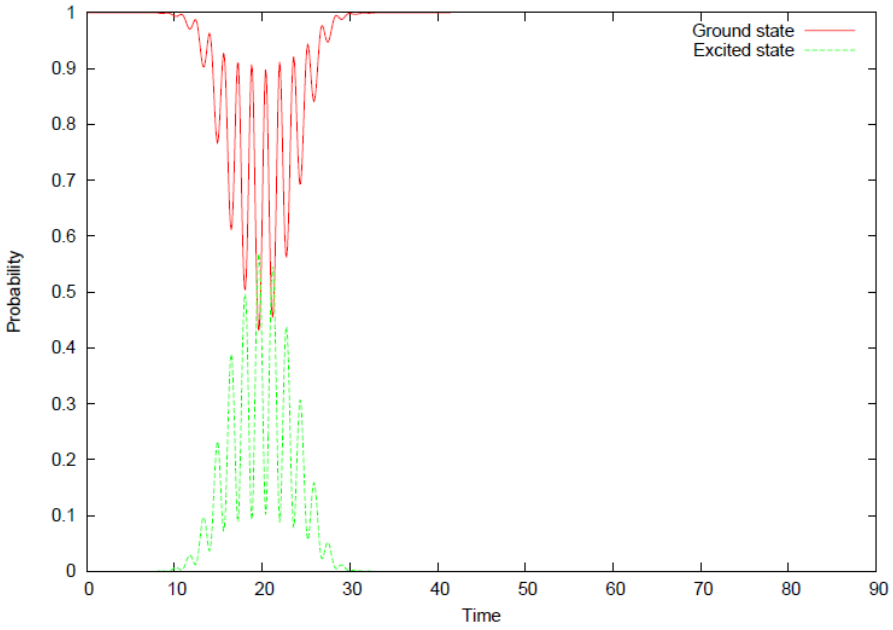
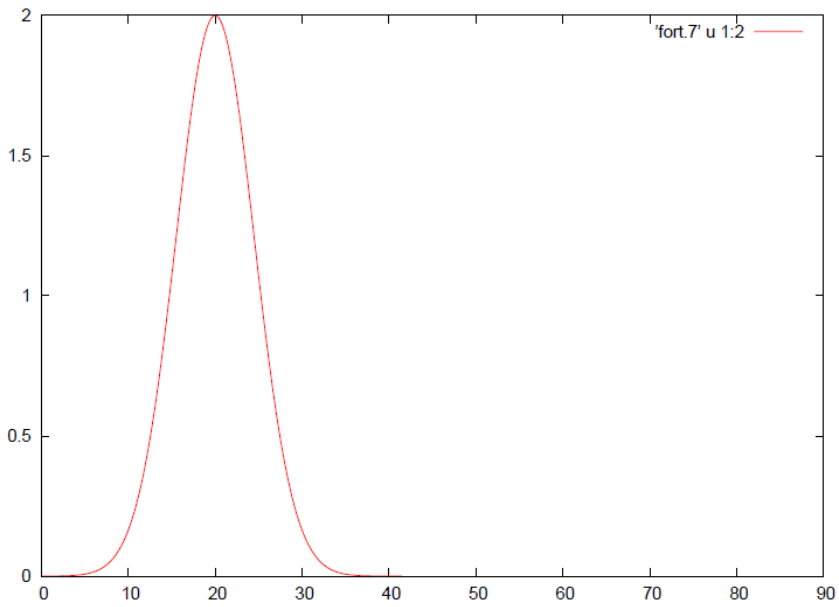


Fig6: Transition Probabilites corresponding to gausian laser pulse shape



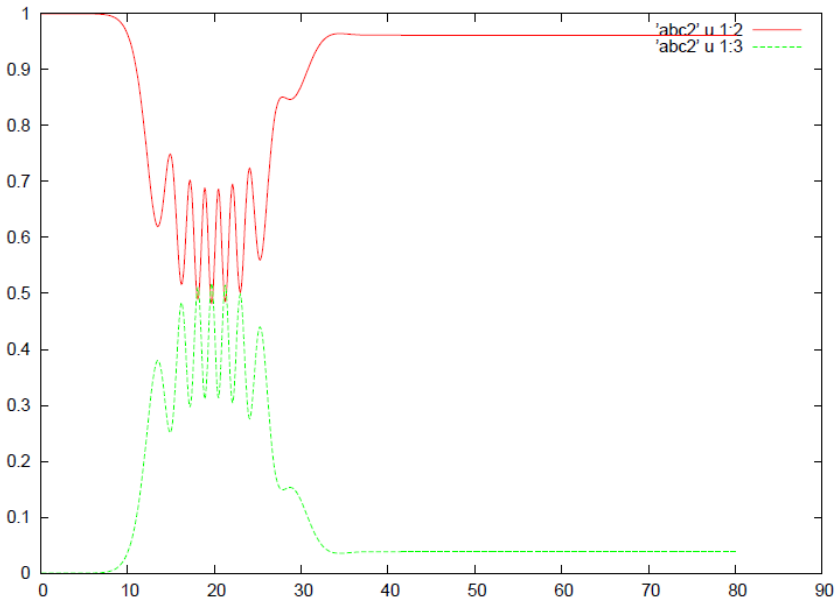


Fig 7 : in the lower figure transitition probabilities are shown on y axis and time in second is shown on x axis, in the above part electric field is represented on y axis and time is represented on x axis for a pulse.

As it can be seen that transition probability appears during which pulse remains non zero.

In conclusion we can solve the coupled equation using Runga Kutta method.

References

1 – Quantum Dots: A Survey of the Properties of Artificial Atoms , Tapash Tackroborty

2- Numerical Methods for Ordinary Differential Equations, J. C. Butcher, john wely sons (2008)