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

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Runge-Kutta Methods

We started with:

$$y_{n+1} = y_n + ak_1 + bk_2$$

$$k_1 = hf\left(x_n, y_n\right)$$

$$k_2 = hf\left(x_n + \alpha h, y_n + \beta k_1\right)$$

a , *b* , *α* and *β* are appropriate weights to be found

Using:

$$a = \frac{1}{2} \quad b = \frac{1}{2}, \quad \alpha = \beta = 1$$

$$k_1 = hf\left(x_i, y_i\right)$$

$$k_2 = hf\left(x_i + h, y_i + k_1\right)$$

$$y_{i+1} = y_i + \frac{1}{2}\left[k_1 + k_2\right]$$

2nd Order Runge-Kutta Method or **Modified Euler's Method**

Runge-Kutta Methods

What if we choose:

the values as $a = \frac{2}{3},\ b = \frac{1}{3},\ \alpha = \frac{3}{2},\ \beta = \frac{3}{2}$

$$y_{i+1} = y_i + ak_1 + bk_2$$

$$k_1 = hf\left(x_i, y_i\right)$$

$$k_2 = hf\left(x_i + \alpha h, y_i + \beta k_1\right)$$

2nd Order Runge-Kutta Method or Heun's Method

Runge-Kutta Methods

Method	Equations
Euler (Error of the order h^2)	$\Delta y = k_1$ $k_1 = h[f(x, y)]$
Modified Euler (Error of the order h^3)	$\Delta y = \frac{1}{2}[k_1 + k_2]$ $k_1 = h[f(x, y)]$ $k_2 = h[f(x + h, y + k_1)]$
Heun (Error of the order h^4)	$\Delta y = \frac{1}{4}[k_1 + 3k_3]$ $k_1 = \Delta h[f(x, y)]$ $k_2 = h\left[f\left(x + \frac{1}{3}h, y + \frac{1}{3}k_1\right)\right]$ $k_3 = h\left[f\left(x + \frac{2}{3}h, y + \frac{2}{3}k_2\right)\right]$
4th order Runge Kutta (Error of the order h^5)	$\Delta y = \frac{1}{6}[k_1 + 2k_2 + 2k_3 + k_4]$ $k_1 = h[f(x, y)]$ $k_2 = h\left[f\left(x + \frac{1}{2}h, y + \frac{1}{2}k_1\right)\right]$ $k_3 = h\left[f\left(x + \frac{1}{2}h, y + \frac{1}{2}k_2\right)\right]$ $k_4 = h[f(x + h, y + k_3)]$

This is a fourth order function that solves an initial value problems using a four step program to get an estimate of the Taylor series through the fourth order.

This will result in a local error of $O(h^5)$ and a global error of $O(h^4)$

The general form of the equations for the 4th Order method are:

$$\Delta y = \frac{1}{6}\left[k_1 + 2k_2 + 2k_3 + k_4\right]$$

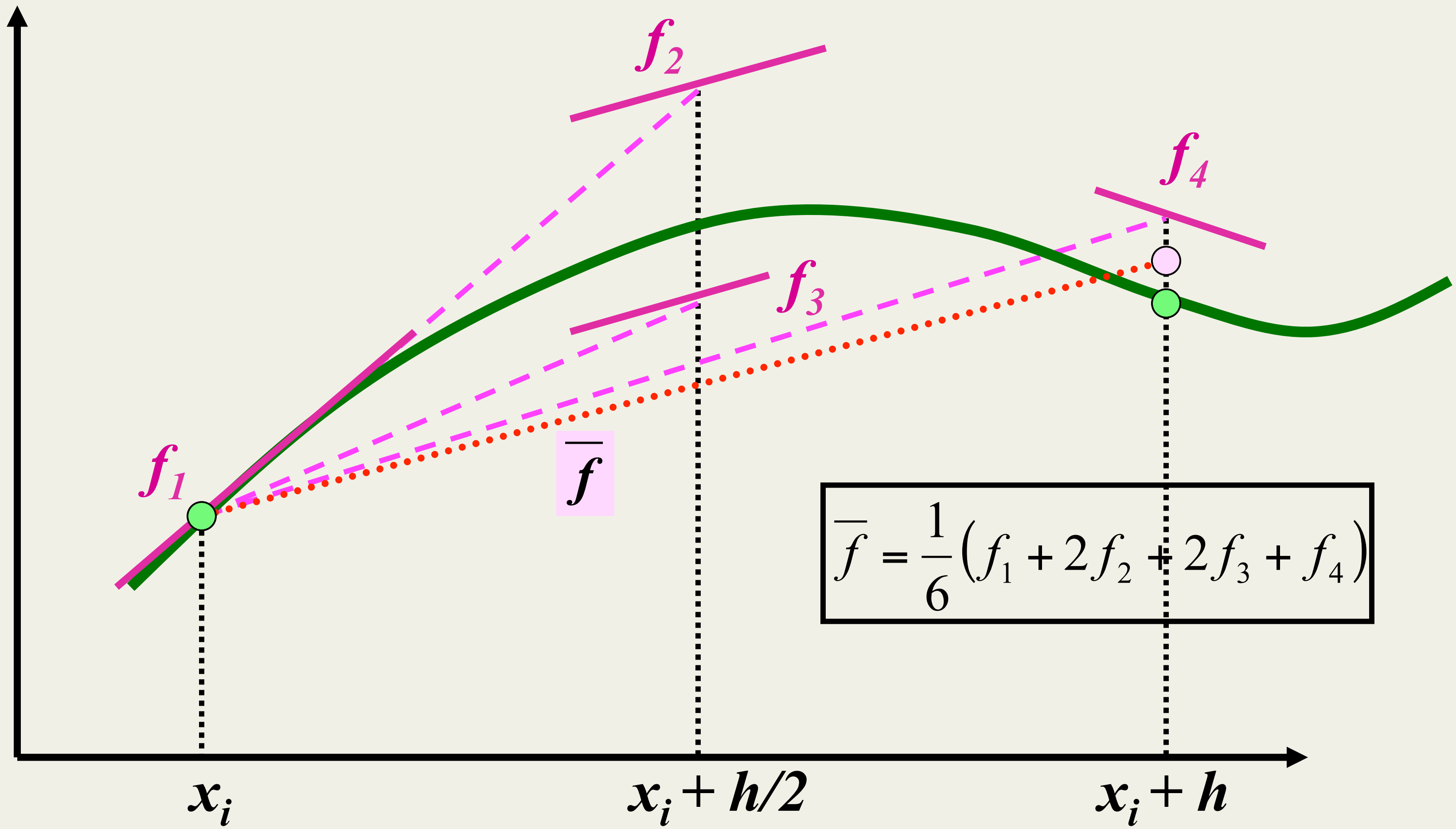
$$k_1 = h\left[f\left(x, y\right)\right]$$

$$k_2 = h\left[f\left(x + \frac{1}{2}h, y + \frac{1}{2}k_1\right)\right]$$

$$k_3 = h\left[f\left(x + \frac{1}{2}h, y + \frac{1}{2}k_2\right)\right]$$

$$k_4 = h\left[f\left(x + h, y + k_3\right)\right]$$

Graphical Representation of the 4rth order method:



How we can solve the coupled equation using this method

The general form of the two equations can be written as follows

$$\frac{dy}{dx} = f\left(x, y, z\right) and \frac{dz}{dx} = g\left(x, y, z\right)$$

with intitial conditions at

$$x = 0, y = y_0, z = z_0$$

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

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

$$k_1^i = f\left(x_i, y_i, z_i\right)$$

$$l_1^i = g\left(x_i, y_i, z_i\right)$$

$$k_2^i = f\left(x_i + \frac{h}{2}, y_i + \frac{k_1^i}{2}, z_i + \frac{l_1^i}{2}\right)$$

$$l_2^i = g\left(x_i + \frac{h}{2}, y_i + \frac{k_1^i}{2}, z_i + \frac{l_1^i}{2}\right)$$

$$k_3^i = f\left(x_i + \frac{h}{2}, y_i + \frac{k_2^i}{2}, z_i + \frac{l_2^i}{2}\right)$$

$$l_3^i = g\left(x_i + \frac{h}{2}, y_i + \frac{k_2^i}{2}, z_i + \frac{l_2^i}{2}\right)$$

$$k_4^i = f\left(x_i + h, y_i + k_3^i, z_i + l_3^i\right)$$

$$l_4^i = g\left(x_i + h, y_i + k_3^i, z_i + l_3^i\right)$$

In the same way we can formulate the solution of n equation

$$\frac{dx}{dt} = f_1(x, y, z, \ldots\ldots, t),$$

$$\frac{dy}{dt} = f_2(x, y, z, \ldots\ldots, t),$$

$$\frac{dz}{dt} = f_3(x, y, z, \ldots\ldots, t)$$

$$t = t_0, x = x_0, y = y_0, z = z_0 \ldots\ldots\ldots$$

Then the solutions can be written as

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

$$y_{i+1} = y_i + \frac{1}{6}\left(l_1^i + 2l_2^i + 2l_3^i + l_4^i\right)h$$

$$z_{i+1} = z_i + \frac{1}{6}\left(m_1^i + 2m_2^i + 2m_3^i + m_4^i\right)h$$

....

....

Where

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

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

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

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

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

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

....

....

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

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

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

....

....

and

$$k_4^i = f_1\left(x_i + k_3^i, y_i + l_3^i, z_i + m_3^i, ..., t_i + h\right)$$

$$l_4^i = f_2\left(x_i + k_3^i, y_i + l_3^i, z_i + m_3^i, ..., t_i + h\right)$$

$$m_4^i = f_3\left(x_i + k_3^i, y_i + l_3^i, z_i + m_3^i, ..., t_i + h\right)$$

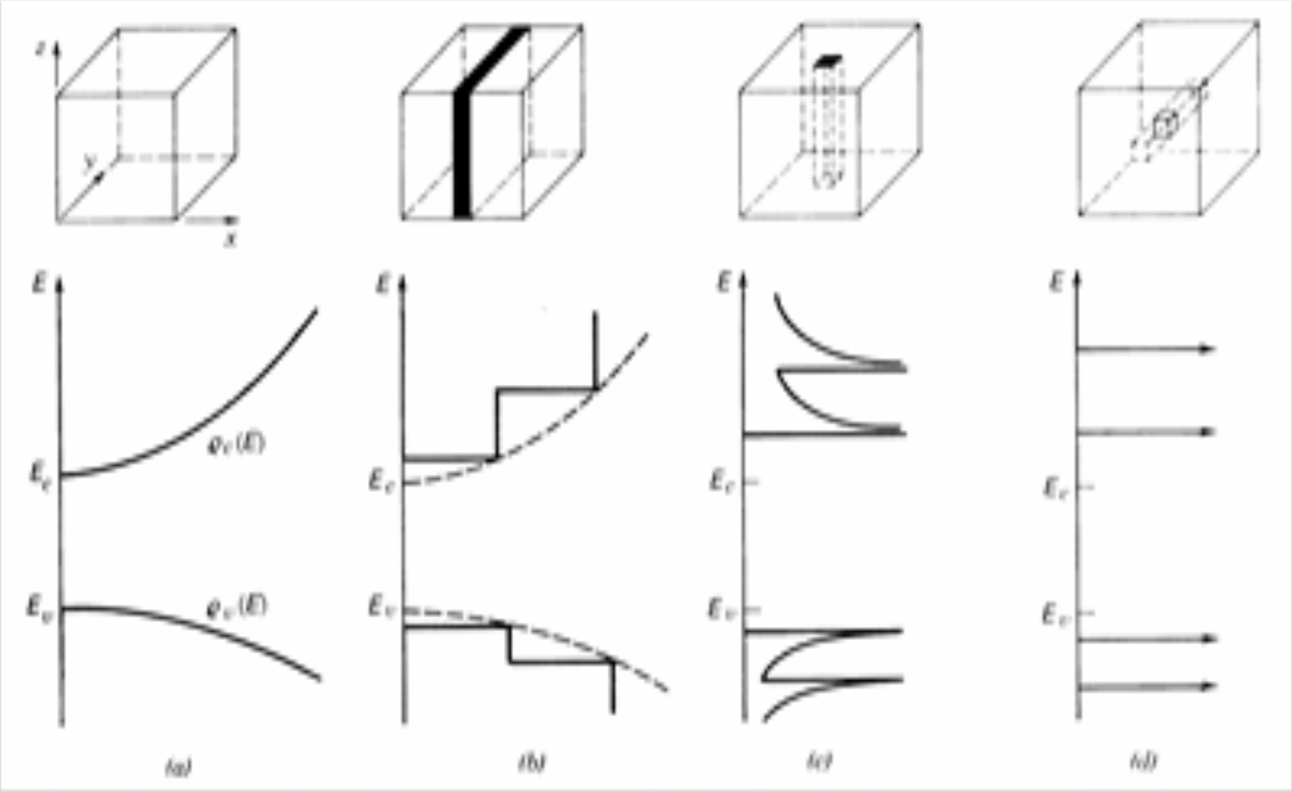
....

....

So we can solve n coupled equations, in the same way we formulate a fortran program of solving n coupled equation , that is

```
      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
```

Laser Pulse effect on Quantum Dot



Finding the eigenenrgies and eigenfunction of Quantum Dot in presence of magnetic field

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

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

$$E_{nl} = (2n + |l| + 1)\hbar\Omega - \frac{\hbar}{2} l \omega_c$$

$$\Omega^2 = \omega_0^2 + \frac{\omega_c^2}{4} \qquad \omega_c = \frac{eB}{m^*} \qquad \Psi_{nl}(\mathbf{r}) = \frac{1}{\sqrt{2\pi}} R_{nl}(r) e^{il\phi}$$

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

$$a = \left(\frac{\hbar}{m^* \Omega}\right)^{1/2}$$

Laser pulse may be form of any shape like Gaussian, rectangular etc. in laser pluse electric field vary with time

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

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

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

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

$\Psi_m(\mathbf{r}, t)$ is the system wave function

m’ denotes particular state having quantum number ‘n,l’ this time dependent wavefunction can be expended in terms of eigenfunction of Hamiltonian H_0 as

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

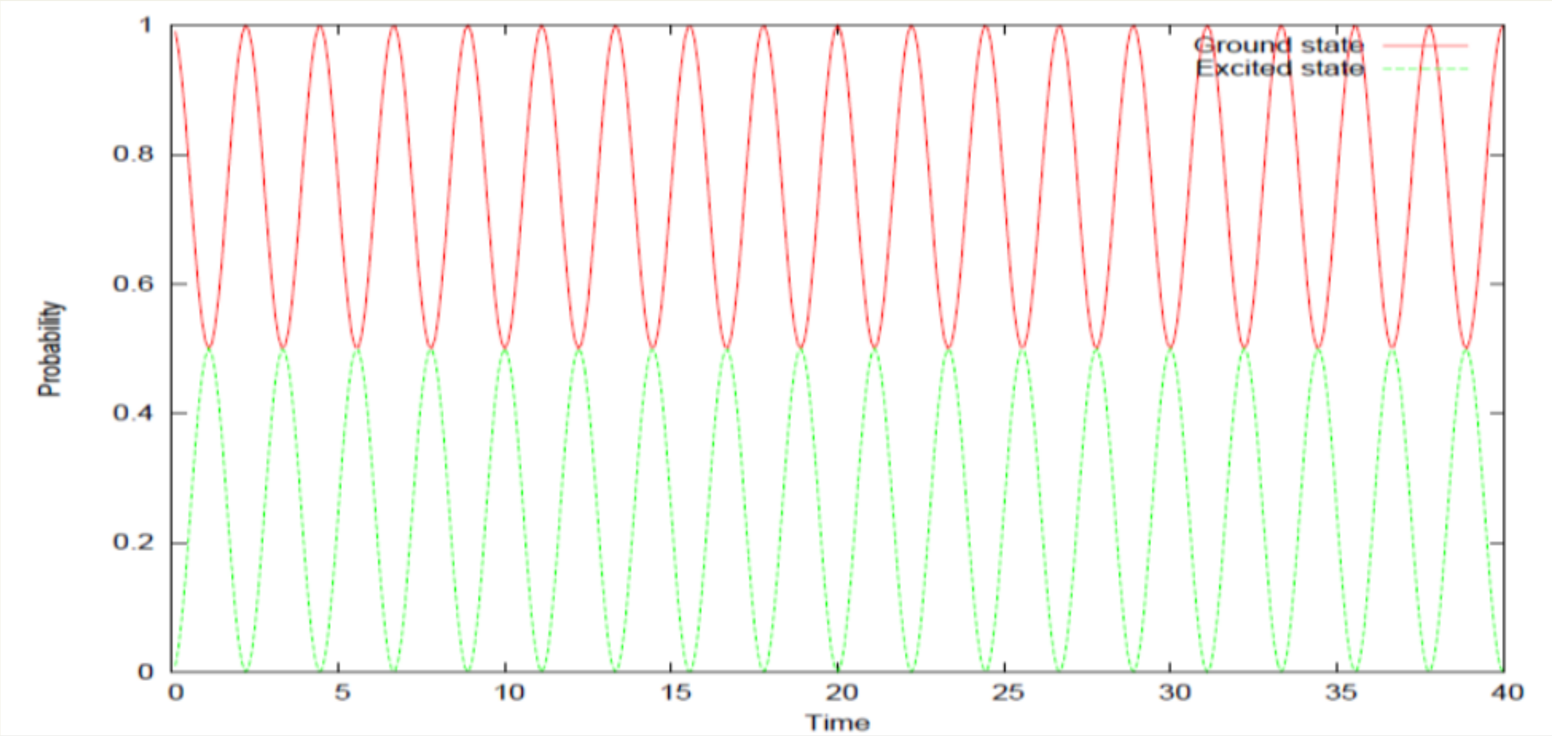
Using the expansion of the wave function $\Psi(\mathbf{r},t)$ and orthogonally of the Eigen states in (14), a set of coupled equation is obtained as

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

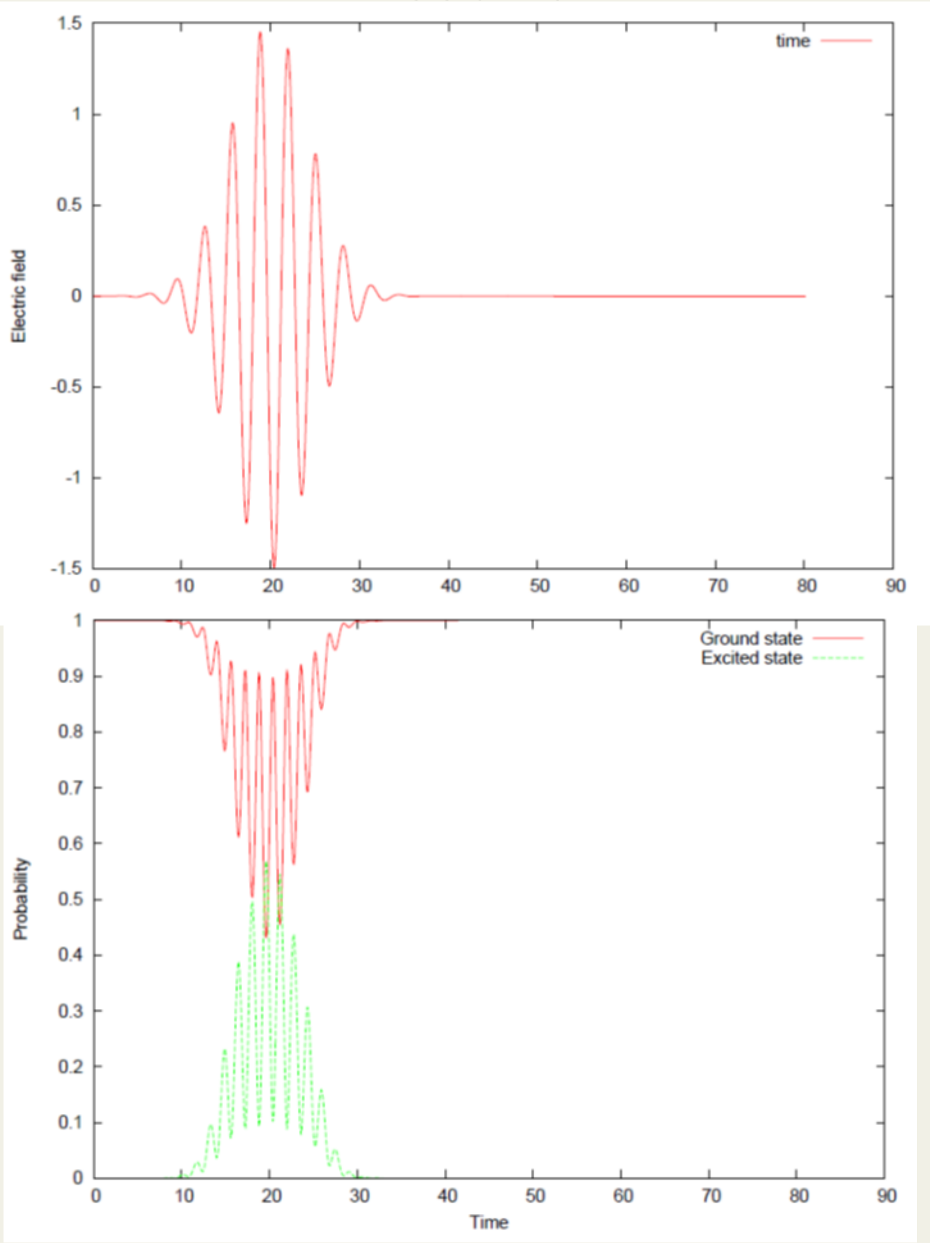
$$\omega_{bk} = \frac{E_b - E_k}{\hbar}$$

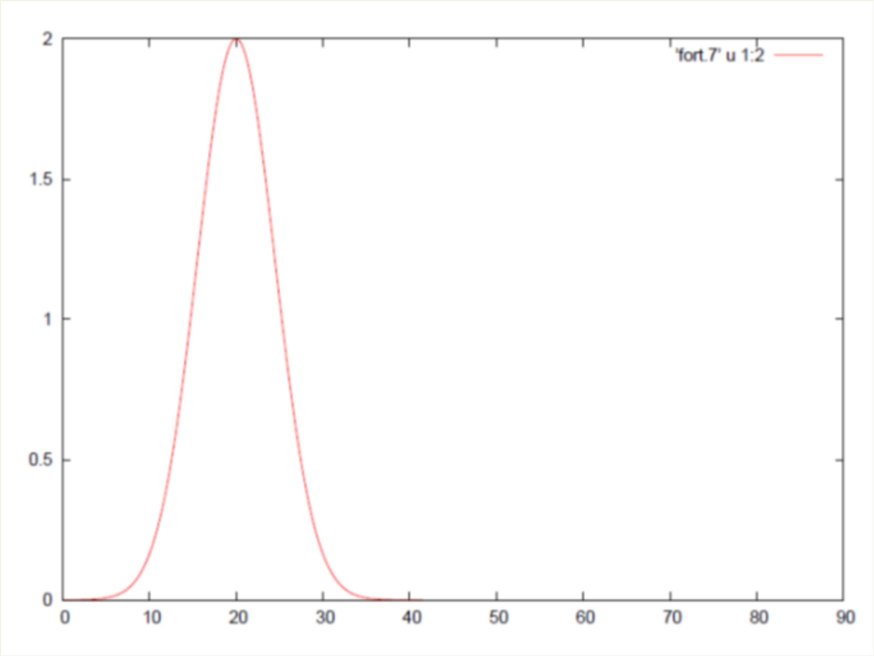
$$i\frac{\partial}{\partial t}c_b(t) = \sum_k \mu_{bk}c_k(t)e^{i\omega_{bk}t}f(t)F_0Cos(\omega t)$$

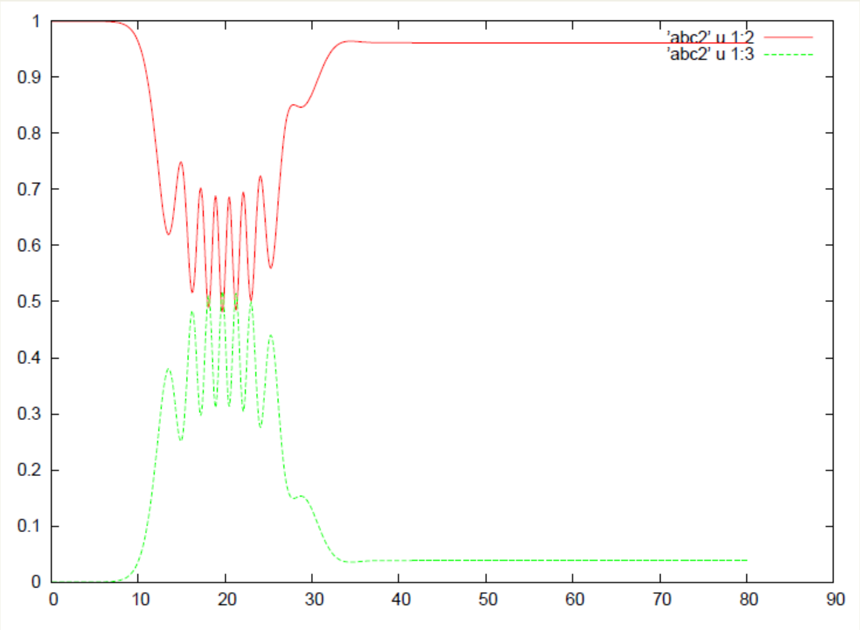
Here $\mu_{bk} = \langle \psi_b | \mathrm{H}_{\mathrm{int}} | \psi_k \rangle = \langle \psi_b | er | \psi_k \rangle$, are the dipole matrix element



Results


time
Electric field
1.5
1
0.5
0
-0.5
-1
-1.5
0
10
20
30
40
50
60
70
80
90
Ground state
Excited state
Probability
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
Time


'fort.7' u 1:2
2
1.5
1
0.5
0
0
10
20
30
40
50
60
70
80
90


'abc2' u 1:2
'abc2' u 1:3
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
0
10
20
30
40
50
60
70
80
90

Thank You