Simulation of a two-level system by mapping spins to springs

Project by

Subrahmanyam Devarakonda

Afreen

Saumitra Singh

Sarthak Mishra

Yashovardhan Jha

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Indian Institute of Science Education and Research

Bhopal, Madhya Pradesh

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ABSTRACT

In this project, we have tried to study the behaviour of the Spin Magnetization Vector of a nucleus subjected to a constant magnetic field on application of Radio Frequency Pulse. For solving the coupled first order differential equations of the trajectory of this vector, we have used the fourth order Runge-Kutta method. We have taken the help of a widely used python Toolbox in Quantum Mechanics called QuTiP to make the simulation of the Spin Magnetization Vector on the Bloch sphere.

ACKNOWLEDGEMENT

We are grateful to Dr. Sunil Pratap Singh for providing us with an opportunity to do a project work where we could explore and apply the theoretical knowledge learnt in the course on a problem of our interest.

We would also like to thank Dr. Subhash Chaturvedi for teaching us the course- Quantum Mechanics in inch perfect details, which helped us in understanding the problem statement and delivering the project to near-perfection.

Contents

1. Nuclear magnetic resonance (NMR)

Nuclear magnetic resonance (NMR) is a physical phenomenon in which nuclei in a strong constant magnetic field are perturbed by a weak oscillating magnetic field and respond by producing an electromagnetic signal with a frequency characteristic of the magnetic field at the nucleus. This process occurs near resonance, when the oscillation frequency matches the intrinsic frequency of the nuclei, which depends on the strength of the static magnetic field, the chemical environment, and the magnetic properties of the isotope involved. NMR results from specific magnetic properties of certain atomic nuclei.

The principle of NMR usually involves three sequential steps:

- The alignment (polarization) of the magnetic nuclear spins in an applied, constant magnetic field B_0.
- The perturbation of this alignment of the nuclear spins by a weak oscillating magnetic field, usually referred to as a radio-frequency (RF) pulse. The oscillation frequency required for significant perturbation is dependent upon the static magnetic field (B_0) and the nuclei of observation.
- The detection of the NMR signal during or after the RF pulse, due to the voltage induced in a detection coil by precession of the nuclear spins around B0. After an RF pulse, precession usually occurs with the nuclei's intrinsic Larmor frequency and, in itself, does not involve transitions between spin states or energy levels.

The two magnetic fields are usually chosen to be perpendicular to each other as this maximizes the NMR signal strength. The frequencies of the time-signal response by the total magnetization (M) of the nuclear spins are analyzed in NMR spectroscopy and magnetic resonance imaging. Both use applied magnetic fields (B_0) of great strength, often produced by large currents in superconducting coils, in order to achieve dispersion of response frequencies and of very high homogeneity and stability in order to deliver spectral resolution, the details of which are described by chemical shifts, the Zeeman effect, and Knight shifts (in metals). The information provided by NMR can also be increased using hyperpolarization, and/or using two-dimensional, three-dimensional and higher-dimensional techniques.

1.1 Theory of nuclear magnetic resonance:

Nuclear spin and magnets

All nucleons, that is neutrons and protons, composing any atomic nucleus, have the intrinsic quantum property of spin, an intrinsic angular momentum analogous to the classical angular momentum of a spinning sphere. The overall spin of the nucleus is determined by the spin quantum number S. If the numbers of both the protons and neutrons in a given nuclide are even then S = 0, i.e. there is no overall spin. Then, just as electrons pair up in non-degenerate atomic orbitals, so do even numbers of protons or even numbers of neutrons (both of which are also spin 1/2 particles and hence fermions), giving zero overall spin.

A non-zero spin **S** is always associated with a non-zero magnetic dipole moment, μ, via the relation

$$\mu = \gamma S$$

where γ is the gyromagnetic ratio.

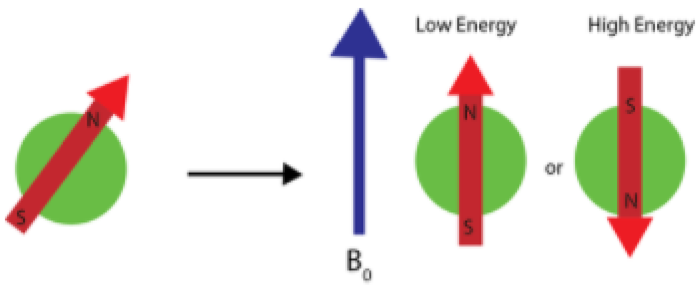
Nuclear spin is an intrinsic angular momentum that is quantized. This means that the magnitude of this angular momentum is quantized (i.e. S can only take on a restricted range of values), and also that the x, y, and z-components of the angular momentum are quantized, being restricted to integer or half-integer multiples of ħ. The integer or half-integer quantum number associated with the spin component along the z-axis or the applied magnetic field is known as the magnetic quantum number, m, and can take values from +S to −S, in integer steps. Hence for any given nucleus, there are a total of 2S + 1 angular momentum states.

The z-component of the angular momentum vector (**S**) is therefore S_z = mħ, where ħ is the reduced Planck constant. The z-component of the magnetic moment is simply:

$$\mu_z = \gamma S_z = \gamma m\hbar$$

1.2 Nuclear Energy Levels

Consider nuclei with a spin of one-half, each nucleus has two linearly independent spin states, with m = ½ or m = -½ (also referred to as spin-up and spin-down, or sometimes α and β spin states, respectively) for the z-component of spin. In the absence of a magnetic field, these states are degenerate; that is, they have the same energy. Hence the number of nuclei in these two states will be essentially equal at thermal equilibrium.



If a nucleus is placed in a magnetic field, however, the two states no longer have the same energy as a result of the interaction between the nuclear magnetic dipole moment and the external magnetic field. The energy of a magnetic dipole moment μ in a magnetic field B_0 is given by:

$$E = -\mu B_0 = -\mu_x B_{0x} - \mu_y B_{0y} - \mu_z B_{0z}$$

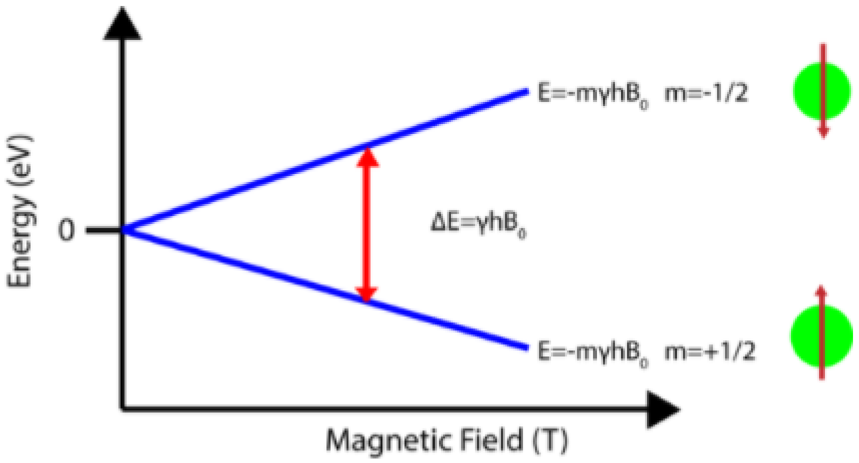
Usually the z-axis is chosen to be along B_0, and the above expression reduces to:

$$E = -\mu_z B_0 = -\gamma m\hbar B_0$$

As a result, the different nuclear spin states have different energies in a non-zero magnetic field. In less formal language, we can talk about the two spin states of a spin ½ as being aligned either with or against the magnetic field. If γ is positive (true for most isotopes used in NMR) then m = ½ is the lower energy state.

The energy difference between the two states is $\Delta E = \gamma\hbar B_0$

and this results in a small population bias favoring the lower energy state in thermal equilibrium. With more spins pointing up than down, a net spin magnetization along the magnetic field B_0 results.



Splitting of nuclei spin energies in an external magnetic field

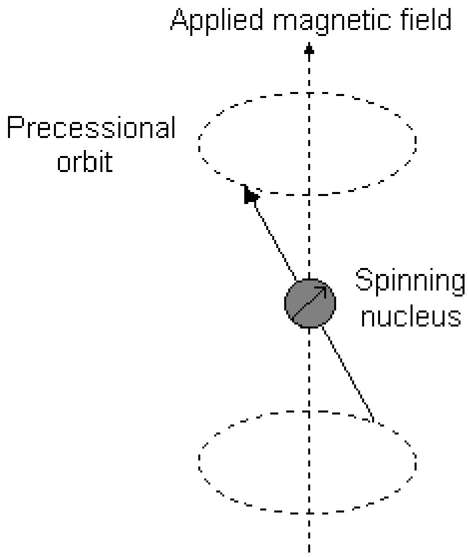
1.3 Energy Transitions (Spin Flip)

A central concept in NMR is the precession of the spin magnetization around the magnetic field at the nucleus, with the angular frequency

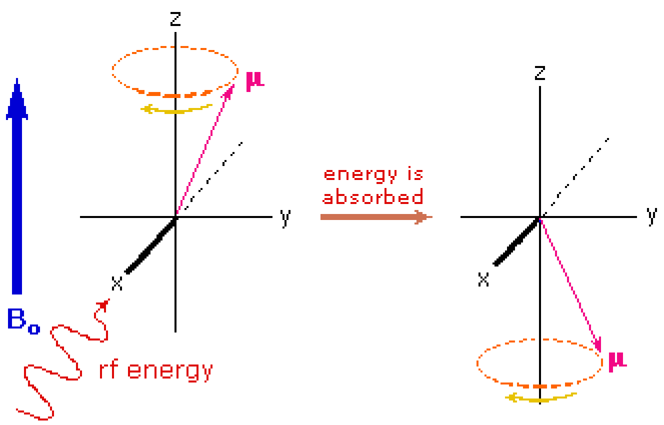
$$\omega = -\gamma B$$

where $\omega = 2\pi\nu$ relates to the oscillation frequency ν and **B** is the magnitude of the field. This means that the spin magnetization, which is proportional to the sum of the spin vectors of nuclei in magnetically equivalent sites, moves on a cone around the **B** field. This is analogous to the precessional motion of the axis of a tilted spinning top around the gravitational field. Precession of non-equilibrium magnetization in the applied magnetic field B_0 occurs with the Larmor frequency

$$\omega_L = 2\pi\nu_L = -\gamma B_0$$



Just as a spinning mass will precess in a gravitational field (a gyroscope), the magnetic moment µ associated with a spinning spherical charge will precess in an external magnetic field. If RF(Radio Frequency) energy having a frequency matching the Larmor frequency is introduced at a right angle to the external field, the precessing nucleus will absorb energy and the magnetic moment will flip from m=1/2 to its m = -1/2 state.



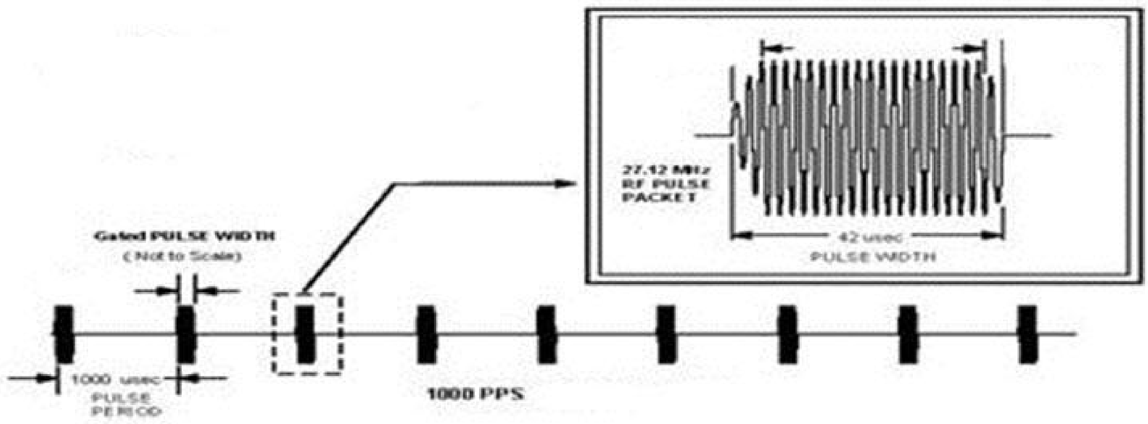
Flip from m=1/2 to m=-1/2 state

2. PULSES

2.1 PULSED RF

Theory:

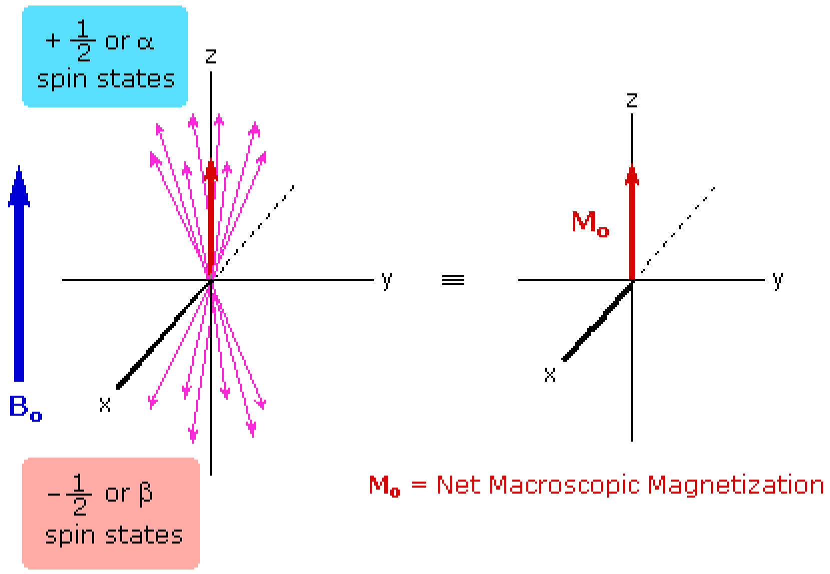
Pulsed radiofrequency is the technique whereby radio frequency (RF) oscillations are gated at a rate of pulses (cycles) per second (one cycle per second is known as a hertz (Hz)). Radio frequency energies occupy 1.0 x 104 Hz to 3.0 x 1011 Hz of the electromagnetic spectrum. Radio frequency electromagnetic energy is routinely produced by RF electrical circuits connected to a transducer, usually an antenna.



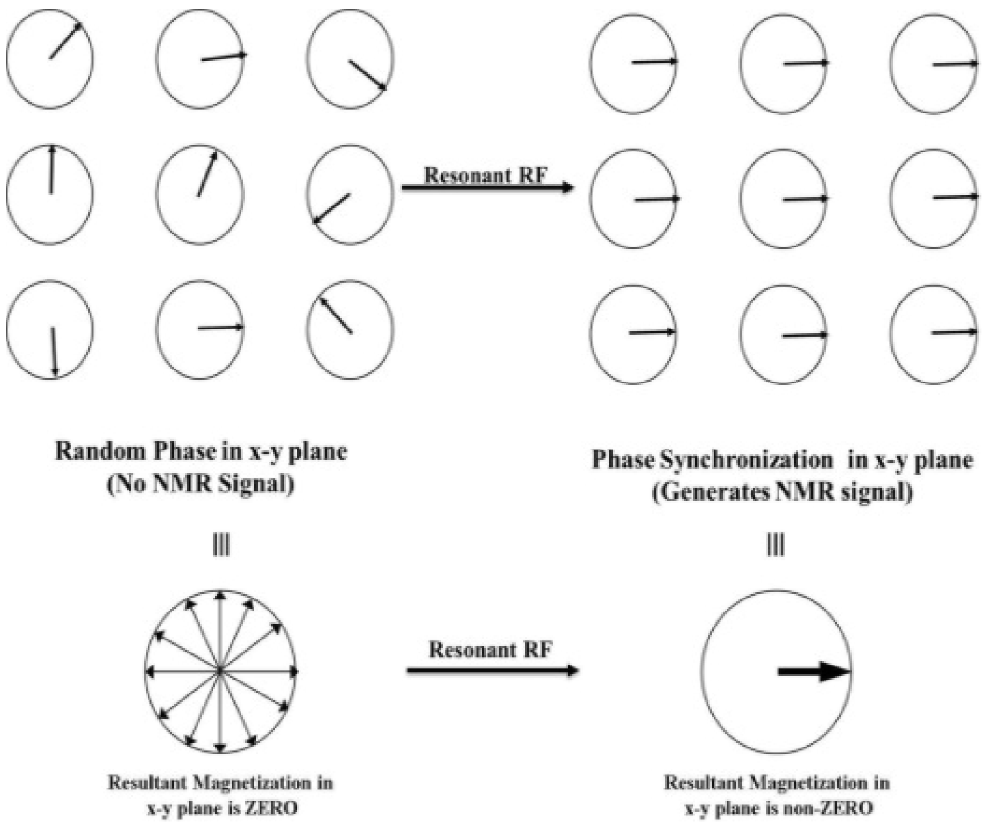
The figure above shows an example of a generalized pulsed radio frequency waveform as seen with an oscilloscope with an antenna probe. In this example there are 1000 pulses per second (one kilohertz pulse rate) with a gated pulse width of 42 µs. The pulse packet frequency in this example is 27.125 megahertz (MHz) of RF energy. The duty cycle for a pulsed radio frequency is the percent time the RF packet is on, 4.2% for this example ([0.042 ms X 1000 pulses divided by 1000 ms/s] X 100). The pulse packet form can be a square, triangle, sawtooth or sine wave. In several applications of pulse radio frequency, such as radar,[2] times between pulses can be modulated.

2.2 Role of RF pulse in NMR:

A rectangular RF (hard) pulse very close to the Larmor frequency and at very high power levels is applied to the probe coil for a short duration (~ 10 µs). Being rectangular in shape, its power instantly reaches to maximum, holds at that level for the entire duration of the pulse, thereafter it instantly goes to zero. The oscillating magnetic field (at a certain phase) rotating in the x − y plane at the frequency of the pulse (close to the Larmor frequency) is created by the pulse. Length of the magnetic field vector of this RF pulse is equal to its amplitude. In NMR spectroscopy these individual spins are 'organized' by the RF pulse so that their individual signals do not just cancel each other out. If all of the vectors representing the magnetic dipoles of the individual spins are lined up in a row, all of them precess in the same direction (counterclockwise) and at exactly the same rate, the Larmor frequency (ν_L). But at equilibrium (random phase), the vectors are located at different points of the circular path. If only the spins in the lower energy (m= ½) state are considered (precessing around a cone facing upward), there is no phase coherence in the ensemble and the random orientations of the precessing spins cancel out their motions (no measurable signal). The RF pulse synchronizes the spins (gets them in phase and generates phase coherence). With this organization of the sample spins extending to the bulk level, the individual magnetic vectors add together to give a bulk magnetic vector (the 'bulk magnetization') of the sample. This vector also rotates counterclockwise at the Larmor frequency around the upper cone at the Larmor frequency.



Net Macroscopic Magnetization of a Sample in an External Magnetic Field B_o



Simplified depiction of the effect of RF on the phase coherence of spins.

3. SIMULATION BY MAPPING SPINS TO SPRINGS

We are going to manipulate the spin magnetization vector of a nucleus by a single control signal.We will perform this task by a sequence of engineered electromagnetic pulses (RF pulses) to produce the time evolution of the given two level system from some given initial state to some desired final state.

The evolution of the two-level system,which is the spin magnetization vector in our case, is described by the Bloch equations.when the frequency of the applied RF pulse is tuned to match the frequency of precession of spin magnetization in a constant magnetic field,which is called the larmor frequency, then the resonance occurs and inversion or rotation of the spin magnetization takes place.

The Bloch equation for the spin magnetization vector are given by-

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} M_x(t,\omega) \\ M_y(t,\omega) \\ M_z(t,\omega) \end{bmatrix} = \begin{bmatrix} 0 & -\omega & u(t) \\ \omega & 0 & -v(t) \\ -u(t) & v(t) & 0 \end{bmatrix} \begin{bmatrix} M_x(t,\omega) \\ M_y(t,\omega) \\ M_z(t,\omega) \end{bmatrix}}$$

$$M_x(\dot{t}, w) = -wM_y(t, w) + u(t)M_z(t, w)$$

$$M_y(\dot{t}, w) = wM_x(t, w) - v(t)M_z(t, w)$$

$$M_z(\dot{t}, w) = -u(t)M_x(t, w) + v(t)M_y(t, w)$$

$$M_x(\dot{t}, w) = -wM_y(t, w) + u(t)M_z(t, w)$$

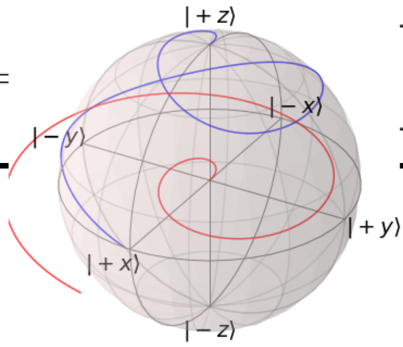
$$M_y(\dot{t}, w) = wM_x(t, w)$$

$$M_z(\dot{t}, w) = -u(t)M_x(t, w)$$

Where Mx,My and Mz are the components of spin magnetization vector M such that ||M|| = 1. w is the larmor frequency of the magnetization vector in a constant magnetic field. u(t) and v(t) are two controls applied in x and y direction respectively.In our case to simplify we are going to deal with only one control along x-direction so we have taken v(t) = 0.

Now consider an undamped harmonic oscillator -

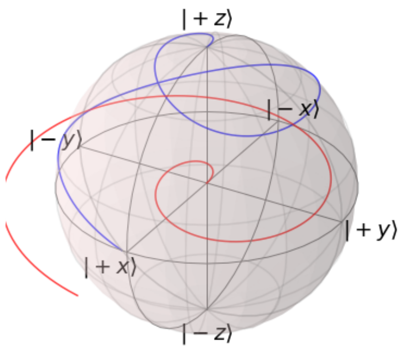
$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} x(t,\omega) \\ y(t,\omega) \end{bmatrix} =$$



$$\Big] + \begin{bmatrix} 1 \\ 0 \end{bmatrix} u\,(t)$$

Where (x,y) ,w and u(t) represent the oscillator's velocity and position,frequency, and external forcing.

From the two boxes above, we can see that when u(t) and v(t) both are zero then the dynamics of the oscillator and transverse magnetization vector (Mx and My) are the same.So this property has been exploited to do the mapping between spring and spin and to calculate the optimum pulse to steer our magnetization vector.The magnetization vector has been steered from M(0)=(0,0,1) to M(T=π)=(1,0,0) and oscillator from (x,y) = (0,0) to (x,y) = (π/2,0).
The optimum pulse that have been calculated to steer both oscillator and magnetization vector from given initial state to given final state is u(t) = -cos(3t)



The blue trajectory corresponds to the spin and red trajectory corresponds to the harmonic oscillator.

4. NUMERICAL ANALYSIS

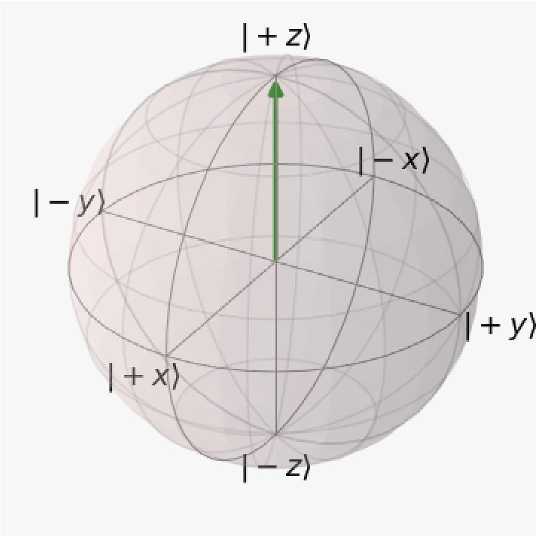
To get the trajectory of the spin magnetization vector we have used the following equations in matrix form-

$$\boxed{\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix} M_x(t,\omega) \\ M_y(t,\omega) \\ M_z(t,\omega) \end{bmatrix} = \begin{bmatrix} 0 & -\omega & u(t) \\ \omega & 0 & -v(t) \\ -u(t) & v(t) & 0 \end{bmatrix}\begin{bmatrix} M_x(t,\omega) \\ M_y(t,\omega) \\ M_z(t,\omega) \end{bmatrix}}$$

We have solved these coupled equations using the fourth order runge kutta method and to plot the trajectory we have used QuTiP(Quantum Toolbox in Python).

5. RESULTS

Here is our final Simulation -



[Click here to view the simulation]

6.Python Code for the Simulation and Trajectory

In [142…
```
from qutip import *
import numpy as np
import matplotlib.pyplot as plt
from pylab import *
import matplotlib.animation as animation
from mpl_toolkits.mplot3d import Axes3D
```

In [143…
```
w = 3 #frequency
```

In [144…
```
T = np.linspace(0,np.pi,1000)
```

In [145…
```
h = (t[-1]-t[0])/1000  #h is the step size
N = len(T)
```

In [146…
```
#Here are the equations for spin trajectory

#Mx' = -w*My+u(t)*Mz
#My' = w*Mx
#Mz' = -u(t)*Mx

#w=3

#M(0) = (0,0,1) initial state
```

In [147…
```
#Now we are defining Mx,My,Mz as arrays
Mx    = np.zeros((N,1))
My    = np.zeros((N,1))
Mz    = np.zeros((N,1))
```

In [148…
```
#Mx1,My1,Mz1 are functions ,
#which will return coupled equations for components
#of spin magnetization vector
```

In [149…
```
def Mx1(t,Mx,My,Mz):
    return -3*My -np.cos(3*t)*Mz
```

In [150…
```
def My1(t,Mx,My,Mz):
    return 3*Mx
```

In [151…
```
def Mz1(t,Mx,My,Mz):
    return np.cos(3*t)*Mx
```

In [152…
```
#Adding the initial condition M(0) = (0,0,1)
```

In [153…
```
Mx[0],My[0],Mz[0] = 0,0,1
```

In [154…

```
#Now defining the function for 4th order runge kutta method
```

In [180…

```
def RK4_3(fx,fy,fz,Cx,Cy,Cz,t):
    for i in range(N-1):

        K1 = h * fx( t[i] , Cx[i], Cy[i] ,  Cz[i]);
        L1 = h * fy( t[i], Cx[i] ,  Cy[i] , Cz[i]);
        M1 = h * fz( t[i] , Cx[i], Cy[i] , Cz[i]);

        K2 = h*fx(t[i]+1/2*h,Cx[i]+1/2*K1 ,Cy[i]+1/2*L1,Cz[i]+1/2*M1);
        L2 = h*fy(t[i]+1/2*h,Cx[i]+1/2*K1 ,Cy[i]+1/2*L1,Cz[i]+1/2*M1);
        M2 = h*fz(t[i]+1/2*h,Cx[i]+1/2*K1 ,Cy[i]+1/2*L1,Cz[i]+1/2*M1);

        K3 = h *fx(t[i]+1/2*h,Cx[i]+1/2*K2,Cy[i]+1/2*L2,Cz[i]+1/2*M2);
        L3 = h *fy(t[i]+1/2*h,Cx[i]+1/2*K2,Cy[i]+1/2*L2,Cz[i]+1/2*M2);
        M3 = h *fz(t[i]+1/2*h,Cx[i]+1/2*K2,Cy[i]+1/2*L2,Cz[i]+1/2*M2);

        K4 = h * fx( t[i]+h ,  Cx[i]+K3, Cy[i]+L3,Cz[i]+M3);
        L4 = h * fy( t[i]+h ,  Cx[i]+K3 , Cy[i]+L3, Cz[i]+M3);
        M4 = h * fz( t[i]+h ,  Cx[i]+K3 , Cy[i]+L3, Cz[i]+M3);

        Cx[i+1] = Cx[i]+1/6*(K1+2*K2+2*K3+K4);
        Cy[i+1] = Cy[i]+1/6*(L1+2*L2+2*L3+L4);
        Cz[i+1] = Cz[i]+1/6*(M1+2*M2+2*M3+M4);

    return Cx,Cy,Cz
```

In [181…

```
Mx,My,Mz = RK4_3(Mx1,My1,Mz1,Mx,My,Mz,T)
```

In [182…

```
Mxx= np.linspace(0,np.pi,1000)
Myy,Mzz = np.linspace(0,np.pi,1000),np.linspace(0,np.pi,1000)
```

In [183…

```
for i in range(len(Mx)):
    Mxx[i] = Mx[i][0]
    Myy[i] = My[i][0]
    Mzz[i] = Mz[i][0]
```

In [184…

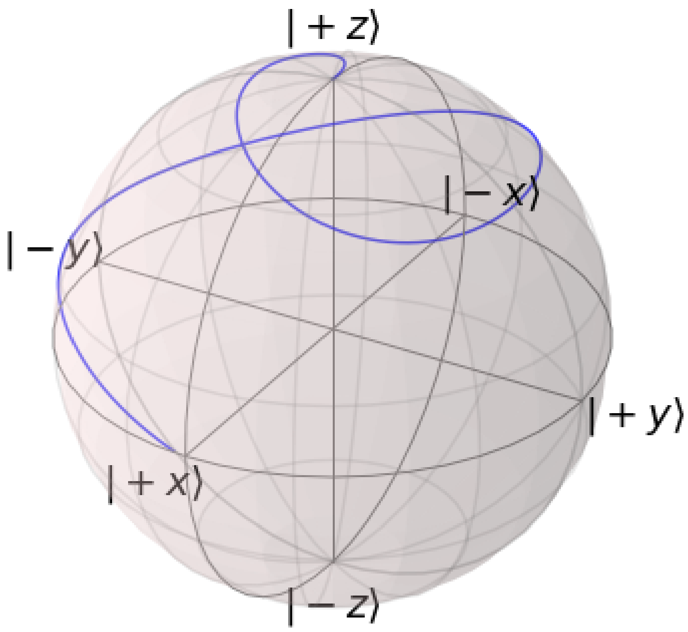
```
B = Bloch()

B.add_points([Mxx,Myy,Mzz], meth = 'l') # adding points for spin trajectory



B.zlabel = ['$\\left|+z\\right>$','$\\left|-z\\right>$']
B.ylabel = ['$\\left|+y\\right>$','$\\left|-y\\right>$']
B.xlabel = ['$\\left|+x\\right>$','$\\left|-x\\right>$']

B.show()
```



In [160…

```
#Now let's solve equations for Spring
#Here are the equations for spring

# x'(t) = -wy(t) -cos(3t)
# y'(t) = w*x(t)
```

In [161…

```
#Ox1,Oy1 are functions , which will return coupled equations for oscillator
```

In [162…

```
def Ox1(t,x,y):
    return -w*y-np.cos(3*t)
```

In [163…

```
def Oy1(t,x,y):
    return w*x
```

In [164…

```
x    = np.zeros((N,1))
y    = np.zeros((N,1))
```

In [165…

```
x[0],y[0] = 0,0  #adding the initial condition (x,y)=(0,0)
```

In [166…

```
#Now defining the RK4 for two coupled equations

def RK4_2(fx,fy,Cx,Cy,t):
    for i in range(N-1):
        K1     = h * fx( t[i]          , Cx[i]        , Cy[i] );
        L1     = h * fy( t[i]          , Cx[i]       ,  Cy[i]);


        K2     = h * fx(t[i] + 1/2*h,  Cx[i]+1/2*K1 , Cy[i]+1/2*L1);
        L2     = h * fy(t[i] + 1/2*h,  Cx[i]+1/2*K1 , Cy[i]+1/2*L1 );
```

```
        K3     = h * fx(t[i] + 1/2*h,  Cx[i] + 1/2*K2 , Cy[i] + 1/2*L2);
        L3     = h * fy(t[i] + 1/2*h,  Cx[i] + 1/2*K2 , Cy[i] + 1/2*L2);


        K4     = h * fx( t[i]+h    ,  Cx[i]+K3     , Cy[i]+L3);
        L4     = h * fy( t[i]+h    ,  Cx[i]+K3     , Cy[i]+L3);


        Cx[i+1] = Cx[i]+1/6*(K1+2*K2+2*K3+K4);
        Cy[i+1] = Cy[i]+1/6*(L1+2*L2+2*L3+L4);


    return Cx,Cy
```

In [167…

```
x,y = RK4_2(Ox1,Oy1,x,y,T)
```

In [168…

```
xx = np.linspace(0,np.pi,1000)
yy,zz=np.linspace(0,np.pi,1000),np.linspace(0,np.pi,1000)
```

In [169…

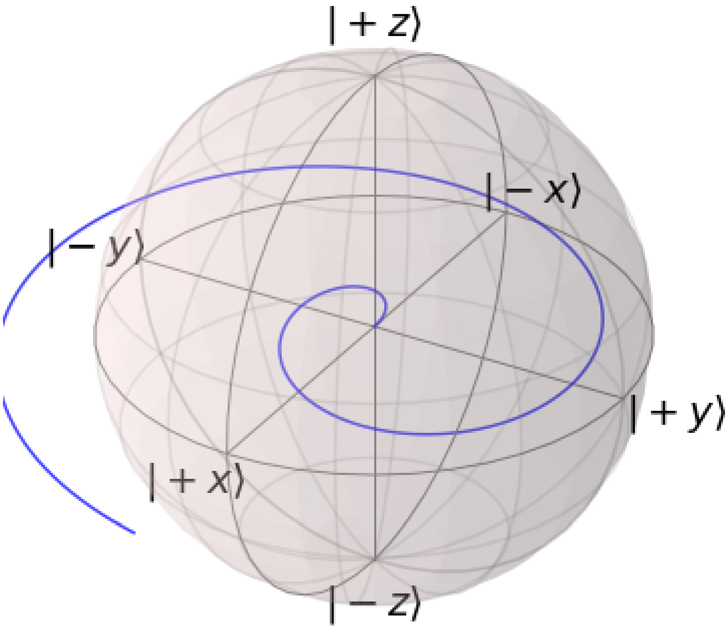
```
for i in range(len(Mx)):
    xx[i] = x[i][0]
    yy[i] = y[i][0]
    zz[i] = 0
```

In [170…

```
B = Bloch()

B.add_points([xx,yy,zz], meth = 'l')   # adding points for spin trajectory
B.zlabel = ['$\\left|+z\\right>$','$\\left|-z\\right>$']
B.ylabel = ['$\\left|+y\\right>$','$\\left|-y\\right>$']
B.xlabel = ['$\\left|+x\\right>$','$\\left|-x\\right>$']

B.show()
```



In [171…

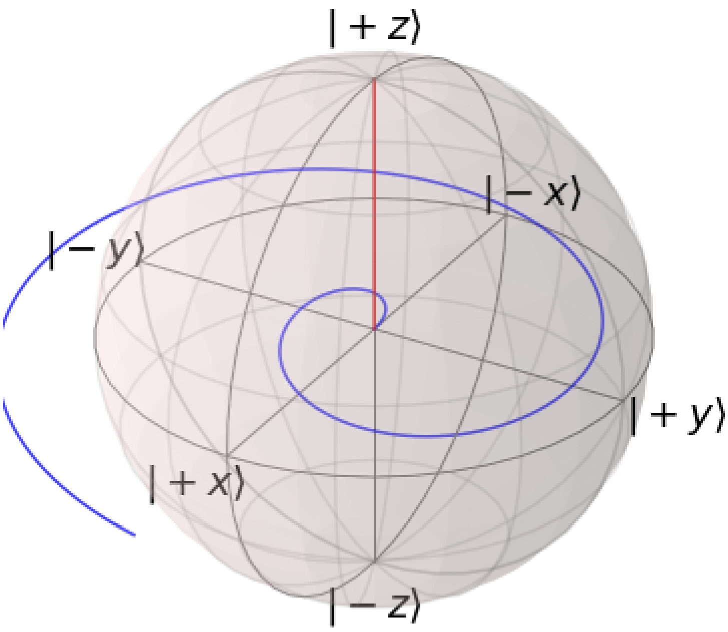
```
B = Bloch()

B.add_points([xx,yy,zz], meth = 'l')

B.add_points([Mxx,Myy,Mzz], meth = 'l')

B.zlabel = ['$\\left|+z\\right>$','$\\left|-z\\right>$']
B.ylabel = ['$\\left|+y\\right>$','$\\left|-y\\right>$']
B.xlabel = ['$\\left|+x\\right>$','$\\left|-x\\right>$']

B.show()
```



In [172…

```
#simulation part
```

In [ ]:

```
fig = figure()
axes = Axes3D(fig,azim=-40,elev=30)
B = Bloch(axes=axes)
B.zlabel = ['$\\left|+z\\right>$','$\\left|-z\\right>$']
B.ylabel = ['$\\left|+y\\right>$','$\\left|-y\\right>$']
B.xlabel = ['$\\left|+x\\right>$','$\\left|-x\\right>$']
def simulate(i):
    B.clear()
    B.add_vectors([Mxx[i],Myy[i],Mzz[i]])
    B.add_points([Mxx[:i+1],Myy[:i+1],Mzz[:i+1]])
    B.make_sphere()
    return axes

def init():
    B.vector_color = ['g']
    return axes

simulation = animation.FuncAnimation(fig, simulate, np.arange(len(Mxx)))
simulation.save('simulation.mp4', fps=60)
```

In [ ]:

References

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