OPTI 571L Lab 2: Bloch Vector Dynamics

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This lab explores the main physical process involved in nuclear magnetic resonance (NMR), which was discovered by I. Rabi in 1938. Later, Bloch and Purcell refined the technique, for which they shared the 1952 physics Nobel Prize. Our terminology (Rabi oscillations, Bloch vectors) comes from NMR. In this lab, you will calculate and plot the dynamics of a Bloch vector for a spin-1/2 particle in a time-varying magnetic field. If you wish, you may extend the lab with analytic calculations of spin flips in a rotating frame of reference.

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I. COMPUTING THE DYNAMICS OF A BLOCH VECTOR

Here we consider a spin-1/2 particle at time $t = 0$ in the initial state $|\psi(0)\rangle = |+\rangle_z$. A magnetic field of constant amplitude but a time-varying direction turns on at time $t = 0$, and the spin state of the particle evolves under the Hamiltonian $H(t) = \frac{1}{2}\hbar\omega_0 \cdot [\vec{\sigma} \cdot \hat{u}(t)]$ (and thus in general, $[H(t), H(t')] \neq 0$). In this expression, ω_0 is a constant frequency (proportional to the magnetic field amplitude and the particle's gyromagnetic ratio), $\vec{\sigma} = [\sigma_x, \sigma_y, \sigma_z]$ is the vector of Pauli spin matrices, and $\hat{u}(t)$ is a time-dependent unit vector with the three components $u_x(t)$, $u_y(t)$, and $u_z(t)$. Because $\hat{u}$ is a unit vector, only 2 of these components are independently adjustable. Write a computer simulation that determines how the state $|\psi(t)\rangle$ evolves under this Hamiltonian, assuming the following conditions:

- Use the basis of eigenstates of σ_z as your representation in specifying all states and operators as vectors and matrices.
- Determine $|\psi(t)\rangle$ at each time step $j\delta t$ between $t = 0$ and $t = n \cdot \delta t$, where $n = 1000$ and j is an integer where $0 \leq j \leq n$. In other words, your calculation will involve 1000 time steps, regardless of the step size δt.
- Let $u_x(t) = A\cos(\Omega t)$, $u_y(t) = A\sin(\Omega t)$, and $u_z(t) = \sqrt{1 - A^2}$. If $A = 0$, then the field is a constant that points in the z direction. A is a real constant that you will specify in your code, with $0 \leq A \leq 1$.

In addition to determining the two components of $|\psi(t)\rangle$ for each time step, calculate the following (for each time step) with your program: $\langle\sigma_x\rangle(t)$, $\langle\sigma_y\rangle(t)$, $\langle\sigma_z\rangle(t)$, $\|\langle\vec{\sigma}\rangle(t)\|$, $\|\,|\psi(t)\rangle\|$. These last two quantities are numerical checks, since each should be approximately equal to 1 for all times if your code is working properly and your assumptions are good. Plot these quantities vs. time on separate graphs.

Try to determine the following:

- the possible values for δt that you can use under various conditions;
- whether or not your results make sense under conditions for which you can determine the exact results (such as $A = 0$, or $A = 1$ and $\Omega = 0$);
- any qualitative differences between conditions where $\Omega << \omega_0$ and $\Omega >> \omega_0$;
- various conditions for which your code breaks down, and possible solutions that help extend the range of validity of your results – note that the numerical approach used in this problem could certainly break down for various combinations of δt, maximum evolution time, and Ω.

Finally, once you are satisfied that your code is working and you understand its range of validity, test various initial conditions, or other time-dependent functions of $\hat{u}$, to help build intuition about the spin dynamics of a spin-1/2 particle in a magnetic field. For example, you could let the magnetic field be the time-dependent function $\vec{B}(t) = B_0 \sin(\Omega t)\hat{y}$, and construct your code to handle this possibility.

Aim to study a few evolution conditions that you believe to be characteristic of a range of various conditions obtainable in this problem. Pay particular attention to conditions that you could not determine analytically, but that help you build intuition about the dynamics of a spin-1/2 particle in a magnetic field.

II. FURTHER EXPLORATION: SPIN FLIPS AND A ROTATING FRAME OF REFERENCE

If you wish, you can now examine a problem similar to that of Part 1, but using a method that obtains an analytic solution for certain special cases. This is not a required part of the lab, since it does not involve computer calculations, but you may work through these problems and create new simulations and plots you wish if you would like to extend the lab by a week. For instance, you can construct code that simulates decoherence by using a density matrix approach to this problem, or think of how to simulate a spin-echo experiment and calculation of the Bloch vector for a many-body system.

Each successive part of the analytical problem below builds on the previous parts unless otherwise stated.

Consider a particle with spin quantum number 1/2 and a gyromagnetic ratio γ. The particle is placed in a magnetic field $\vec{B}(t)$, which takes the form

$$\vec{B}(t) = B_z\hat{z} + B_r(\cos(\omega t)\hat{x} + \sin(\omega t)\hat{y}).$$

B_z and B_r are constant magnetic field values for the different components of the total field. The Hamiltonian for the particle is $\hat{H}(t) = -\vec{M}\cdot\vec{B}(t)$, where $\vec{M} = \gamma\vec{S}$ is the particle's magnetic dipole moment operator, and $\vec{S}$ is the usual vector of spin-1/2 operators.

(a) Defining $\omega_0 = -\gamma B_z$ and $\Omega_0 = -\gamma B_r$, write $\hat{H}(t)$ in terms of ω_0, Ω_0, ω, t, and the Pauli spin operators.

(b) Assuming the standard representation of eigenstates of $\hat{S}_z$, write the matrix form of $\hat{H}(t)$. (You are to use this representation for the remaining parts of this problem.)

The goal in rest of this problem is to work through the main part of a method to calculate $|\psi(t)\rangle$, the particle's time-dependent spin state, given $|\psi(0)\rangle$. The difficulty we are faced with is that $[\hat{H}(t), \hat{H}(t')] \neq 0$ for times $t \neq t'$, making the evolution operator difficult to calculate. There is a very nice way to deal with this difficulty: we can make a transformation from the laboratory frame of reference into a reference frame that is co-rotating with the magnetic field direction. Conceptually, this is similar to the reference frame change that you would naturally assume if you were to jump onto a rotating merry-go-round: the merry-go-round itself looks still to you when you are on it, but rotating when you are on the ground. A rotating-frame transformation is straightforward mathematically, and you will be guided through some basic steps below.

First, we will introduce a new quantum state $|\widetilde{\psi}(t)\rangle = R_z^\dagger(\omega t)\,|\psi(t)\rangle$, where $R_z^\dagger(\omega t)$ is the Hermitian conjugate of the spin-1/2 rotation operator $R_z(\omega t)$ as it was defined in class. IF it turns out that we can find $|\widetilde{\psi}(t)\rangle$ given some initial state $|\psi(0)\rangle$, then determining $|\psi(t)\rangle$ is easy: $|\psi(t)\rangle = R_z(\omega t)\,|\widetilde{\psi}(t)\rangle$.

(c) Write $R_z^\dagger(\omega t)$ as an operator in exponential form, and also as a matrix assuming the standard spin-state representation for a spin-1/2 particle. Keep careful track of your signs!

(d) Let $|\psi(t)\rangle = a_+(t)\,|+\rangle + a_-(t)\,|-\rangle$, where $\hat{S}_z|+\rangle = \frac{\hbar}{2}|+\rangle$ and $\hat{S}_z|-\rangle = -\frac{\hbar}{2}|-\rangle$. Also let $|\widetilde{\psi}(t)\rangle = b_+(t)\,|+\rangle + b_-(t)\,|-\rangle$. With $|\widetilde{\psi}(t)\rangle = R_z^\dagger(\omega t)\,|\psi(t)\rangle$, write $b_+(t)$ and $b_-(t)$ in terms of $a_+(t)$, $a_-(t)$, t, and ω.

(e) You should immediately see that $|b_+(t)|^2 = |a_+(t)|^2$ and $|b_-(t)|^2 = |a_-(t)|^2$ (if not, re-check your work!), so if all we care about are the time-dependent probabilities of finding the particle in the $|+\rangle$ or $|-\rangle$ states, then we won't even need to transform back to the non-rotating frame of reference (that is, we *wouldn't* need to calculate $|\psi(t)\rangle$ once we know $|\widetilde{\psi}(t)\rangle$). We can also write the Schrödinger Equation for the rotating frame:

$$i\hbar\frac{d}{dt}|\widetilde{\psi}(t)\rangle = \widetilde{H}(t)|\widetilde{\psi}(t)\rangle,$$

where $\widetilde{H}(t)$ is the Hamiltonian for the rotating frame. Starting with this equation, and using $|\widetilde{\psi}(t)\rangle = R_z^\dagger(\omega t)\,|\psi(t)\rangle$, show that

$$\widetilde{H}(t) = R_z^\dagger(\omega t)\hat{H}(t)R_z(\omega t) - \omega\hat{S}_z.$$

(f) Write the matrix form of $\widetilde{H}(t)$. You should get a relatively simple, time-independent result.

(g) Calculate the matrix form of the rotating-frame time evolution operator $\widetilde{U}(t,0)$ corresponding to evolution of the spin state $|\widetilde{\psi}(t)\rangle$ under the Hamiltonian $\widetilde{H}(t)$. This is obtained via the usual methods, but with $\widetilde{H}$ instead of $H(t)$.

(h) Suppose that at $t = 0$ the spin state $|\psi(t = 0)\rangle$ of the particle is known. Also at $t = 0$, the magnetic field $\vec{B}(t)$ is turned on. Letting $|\psi(t = 0)\rangle = |+\rangle$, and assuming that the spin state of the particle is to be measured at time t, calculate the probability $P_-(t)$ that the particle will be found in state $|-\rangle$ at a later time t. Write your answer in terms of Ω_0, Δ, and t, where $\Delta \equiv \omega - \omega_0$.

(i) Plot $P_-(t)$ vs. t for two cases: $\Delta = 0$ and $\Delta = 3\Omega_0$. Label your plots appropriately.

(j) Let $\max(P_-)$ designate the maximum amplitude of probability oscillations for finding the particle in state $|-\rangle$, for a given set of parameters Δ and Ω_0. An observation of the particle in the $|-\rangle$ state would indicate what we will call a spin-flip transition. With $|\psi(0)\rangle = |+\rangle$, plot $\max(P_-)$ vs. Δ over the range $\Delta = -5\Omega_0$ to $\Delta = 5\Omega_0$.

(k) Consider $P_-(t)$ for the resonance condition $\omega = \omega_0$. In this case, B_r can be arbitrarily small and still cause a spin-flip transition. (In other words, the rotating part of the field can be a minor perturbation to the z-component part of the field — this is usually the case.) However, the shortest time to induce a transition (a π pulse) gets longer with smaller B_r. Plot the time needed for a π-pulse as a function of B_r.

(l) The gyromagnetic ratio for a proton is $\gamma = 2.7 \times 10^4 (\mathrm{s\,G})^{-1}$, where G is the magnetic field dimensional unit Gauss. The strength of the earth's magnetic field at the earth's surface is about 0.75 G. Now suppose that the proton at the center of a hydrogen atom is known to be in the spin state $|+\rangle$ at time $t = 0$. The atom is subject to the earth's static magnetic field (pointing in the z direction), as well as a second field with magnitude 0.01 G rotating in the x, y plane at angular frequency ω. Give a numerical value for ω that would induce a resonant spin-flip transition for the proton, and specify the time needed for a π pulse.

(m) If instead of the magnetic field values given above we used $B_z = 10^4$ G, and $B_r = 100$ G, what would be the resonant frequency for a spin-flip transition and the time that corresponds to a π-pulse?