Rabi Oscillation

Byeongkeun Ahn

March 25, 2019

1   Single qubit: Introduction to spin system

1.1   The two-state nature of spin system

TODO: Bloch-sphere representation, Pauli matrices

We will use the convention that denotes up- and down- spin basis states with respect to the z-axis.

1.2   Schrödinger equation

The interaction energy of magnetic moment $\vec{M}$ within magnetic field $\vec{B} = (B_x, B_y, B_z)$ is given by

$$E = -\vec{M} \cdot \vec{B}. \tag{1}$$

By analogy, we can infer the Hamiltonian of the same system would be given by

$$H = -\vec{M} \cdot \vec{B} = g\vec{S} \cdot \vec{B}, \tag{2}$$

where the kinetic energy has been omitted for brevity and $\vec{M} = -g\vec{S}$ assuming the particle is negatively charged. Here $\vec{S} = (S_x, S_y, S_z)$ is the spin angular momentum operator that satisfies the commutation relation

$$[S_\mu, S_\nu] = i\hbar\epsilon_{\mu\nu\lambda}S_\lambda. \tag{3}$$

The relation (3) originates from the characterization of the angular momentum operator, which reflects the non-commutativity of rotation in 3D space. Although the spin has only two components in its state description, it has complex-valued components that gives rise to three degree-of-freedom except the unobservable phase factor.[1]

The Schrödinger equation describing the time evolution of this system is given by

$$i\hbar\frac{\mathrm{d}\psi}{\mathrm{d}t} = H\psi. \tag{4}$$

---

[1] There is one exception regarding the phase angle that creates some important quantum-mechanical effects. This will be treated later on.

1.3 Equivalence to the classical problem

The equation (4) can be quite complicated to solve, so a good strategy would be to get some intuition by analyzing the same system in the regime of classical mechanics.

Let's see how the expectation value of spin angular momentum evolves in time:

$$\frac{\mathrm{d}\langle S_x \rangle}{\mathrm{d}t} = \frac{\mathrm{d}}{\mathrm{d}t} \psi^\dagger S_x \psi$$
$$= \frac{\mathrm{d}\psi^\dagger}{\mathrm{d}t} S_x \psi + \psi^\dagger S_x \frac{\mathrm{d}\psi}{\mathrm{d}t}$$

Since

$$\frac{\mathrm{d}\psi^\dagger}{\mathrm{d}t} = \left(\frac{1}{i\hbar} H \psi \right)^\dagger = -\frac{1}{i\hbar} \psi^\dagger H^\dagger = -\frac{1}{i\hbar} \psi^\dagger H,$$

the above expression reduces to

$$= -\frac{1}{i\hbar} \psi^\dagger H S_x \psi + \psi^\dagger S_x \frac{1}{i\hbar} H \psi$$
$$= \frac{1}{i\hbar} \psi^\dagger [S_x, H] \psi \tag{5}$$
$$= \frac{1}{i\hbar} \langle [S_x, H] \rangle$$

which is the well-known Ehrenfest's theorem. Now, using the commutation relation (3) we obtain

$$[S_x, H] = g[S_x, S_x B_x + S_y B_y + S_z B_z]$$
$$= g(B_y[S_x, S_y] - B_z[S_x, S_z]) \tag{6}$$
$$= g(B_y i\hbar S_z - B_z i\hbar S_y)$$
$$= -gi\hbar(S_y B_z - S_z B_y)$$

which results in

$$\frac{\mathrm{d}\langle S_x \rangle}{\mathrm{d}t} = -g(\langle S_y \rangle B_z - \langle S_z \rangle B_y) = -g(\langle \vec{S} \rangle \times \vec{B})_x. \tag{7}$$

Repeating the same procedure for y and z, we can obtain

$$\frac{\mathrm{d}\langle \vec{S} \rangle}{\mathrm{d}t} = -g\langle \vec{S} \rangle \times \vec{B}, \tag{8}$$

which is in exactly the same form as the classical equation of motion. The reason why the classical equation of motion is completely recovered is because the three components of the expectation value capture all the necessary information contained in ψ. Hence, our macroscopic tools and intuition can be applied without error for the analysis of spin motion.

2 Larmor Precession

3 Rabi Oscillation

So far we've studied the case where the external magnetic field is static. But what happens if we apply an oscillating field? Let's examine the problem for a simple case called Rabi oscillation, where the field rotates in space as $\vec{B}(t) = (B_\perp \cos(\omega t), B_\perp \sin(\omega t), B)$.

3.1 Frame rotation in classical mechanics

Since the external magnetic field $\vec{B}$ is rotating around the z-axis, it would be natural to analyze the motion in the rotating frame where the field looks static. Let $\vec{S'}$ and $\vec{B'}$ be the angular momentum and the magnetic field viewed in the frame rotating around the z-axis with angular velocity ω. Then

$$\vec{B}(t) = R_z(\omega t)\vec{B'}(t)$$
$$\vec{S}(t) = R_z(\omega t)\vec{S'}(t) \tag{9}$$

where $R_z(\omega t)$ denotes the matrix of rotation around the z-axis by angle ωt. The equation of motion then becomes

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(R_z(\omega t)\vec{S'}\right) = -g\left(R_z(\omega t)\vec{S'}\right) \times \left(R_z(\omega t)\vec{B'}\right) = -gR_z(\omega t)(\vec{S'} \times \vec{B'}) \tag{10}$$

Taking $R_z(-\omega t)$ to the left of both sides

$$\left[R_z(-\omega t)\frac{\mathrm{d}}{\mathrm{d}t}R_z(\omega t)\right]\vec{S'} + \frac{\mathrm{d}\vec{S'}}{\mathrm{d}t} = -g\vec{S'} \times \vec{B'}$$

and by rearranging terms we obtain the equation of motion in the rotating frame

$$\frac{\mathrm{d}\vec{S'}}{\mathrm{d}t} = \left[\left(g\vec{B'} \times\right) - R_z(-\omega t)\frac{\mathrm{d}}{\mathrm{d}t}R_z(\omega t)\right]\vec{S'} \tag{11}$$

where we can see the additional fictitious term involving R_z appearing. Now, the new equation of motion is generally no easier to solve than the original equation. However, in the case of Rabi oscillation, the time evolution operator of $\vec{S'}$ becomes constant:

$$\vec{B'} = R_z(-\omega t)(B_\perp \cos(\omega t), B_\perp \sin(\omega t), B)$$
$$= B\hat{z} + B_\perp \hat{x} \tag{12}$$

$$R_z(-\omega t)\frac{\mathrm{d}}{\mathrm{d}t}R_z(\omega t) = \begin{pmatrix} \cos(\omega t) & -\sin(\omega t) & 0 \\ \sin(\omega t) & \cos(\omega t) & 0 \\ 0 & 0 & 1 \end{pmatrix}\begin{pmatrix} -\omega\sin(\omega t) & -\omega\cos(\omega t) & 0 \\ \omega\cos(\omega t) & -\omega\sin(\omega t) & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$= \omega\begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} = \omega\hat{z} \times \tag{13}$$

Hence the equation of motion simplifies to

$$\frac{\mathrm{d}\vec{S'}}{\mathrm{d}t} = \left[\left(g\vec{B'}\times\right) - (\omega\hat{z}\times)\right]\vec{S'} = (gB_\perp, 0, gB - \omega) \times \vec{S'} \tag{14}$$

which is just an ordinary Larmor precession around a fixed axis. But the axis is different from the axis of rotation we've used in the previous section. To simplify the analysis, let

$$(gB_\perp, 0, gB - \omega) \equiv \omega_p(\sin\alpha, 0, \cos\alpha) \tag{15}$$

and rotate $\vec{S'}$ around the y-axis by angle $-\alpha$:

$$\vec{S''} = R_y(-\alpha)\vec{S'}. \tag{16}$$

Taking $R_y(-\alpha)$ on both sides of (14) and simplifying we obtain

$$\frac{\mathrm{d}\vec{S''}}{\mathrm{d}t} = \omega_p\hat{z} \times \vec{S''} \tag{17}$$

whose solution we know from the previous section

$$\vec{S''}(t) = R_z(\omega_p t)\vec{S''}(0). \tag{18}$$

From (18), we can recover the original vector $\vec{S}$:

$$\begin{aligned}
\vec{S}(t) &= R_z(\omega t)\vec{S'}(t) \\
&= R_z(\omega t)R_y(\alpha)\vec{S''}(t) \\
&= R_z(\omega t)R_y(\alpha)R_z(\omega_p t)\vec{S''}(0) \\
&= R_z(\omega t)R_y(\alpha)R_z(\omega_p t)R_y(-\alpha)\vec{S'}(0) \\
&= R_z(\omega t)R_y(\alpha)R_z(\omega_p t)R_y(-\alpha)\vec{S}(0).
\end{aligned} \tag{19}$$

The motion is superposition of two rotations of different frequencies ω and ω_p with respect to different axes.

Now, let's take a look at a special case, where $\omega = gB$. Then $\alpha = \pi/2$. Since $R_y(\pi/2)R_z(\omega_p t)R_y(-\pi/2) = R_x(\omega_p t)$,

$$\vec{S} = R_z(\omega t)R_x(\omega_p t)\vec{S}(0).$$

The vector rotates with respect to the x-axis and then the z-axis. We can obtain some intuition by examining the following extreme cases:

- $\vec{S}(0) = S\hat{z}$. $\vec{S}$ rotates around the x-axis in the yz-plane when viewed in the rotating frame.

- $\vec{S}(0) = S\hat{x}$. $\vec{S}(t)$ looks like an ordinary Larmor precession around the z-axis, since $\vec{S}(0)$ is not affected by $R_x(\omega_p t)$.
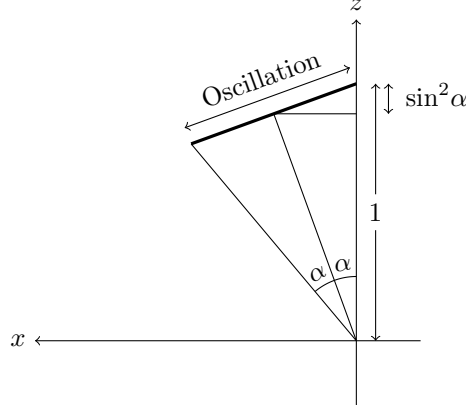
Figure 1: Projection of $\vec{S'}(t)$ onto xz-plane (ignoring $R_z(\omega t)$), denoted with thick line segment

Often we're only concerned with S_z, not the azimuthal angle components (S_x or S_y). In such scenarios we can safely neglect $R_z(\omega t)$ (since it does not touch the z component) and just care about $\vec{S'}(t)$. Let us further restrict our attention to the case $\vec{S'}(0) = \vec{S}(0) = S\hat{z}$ for simplicity. Then $\vec{S'}$ oscillates through a circle centered at $(\sin\alpha\cos\alpha, 0, \cos^2\alpha)$ with radius $\sin\alpha$, as shown in Figure 1.

Hence

$$
\begin{aligned}
S_z(t) &= 1 - \sin^2\alpha\,(1 - \cos\omega_p t) \\
&= 1 - 2\sin^2\alpha\,\sin^2\frac{\omega_p t}{2} \\
&= 1 - 2\,\frac{(gB_\perp)^2}{(gB_\perp)^2 + (gB - \omega)^2}\,\sin^2(\frac{\sqrt{(gB_\perp)^2 + (gB - \omega)^2}}{2}\,t).
\end{aligned}
\tag{20}
$$

As we will see later, $S_z(t)$ corresponds to the probability difference of observing up-spin and down-spin. Hence the initially-up spin state oscillates to give the down-spin probability of

$$
p_\downarrow(t) = \frac{(gB_\perp)^2}{(gB_\perp)^2 + (gB - \omega)^2}\,\sin^2(\frac{\sqrt{(gB_\perp)^2 + (gB - \omega)^2}}{2}\,t).
\tag{21}
$$

3.2   Frame rotation in quantum mechanics

Let's start by writing the Schrödinger equation for our system,

$$
i\hbar\frac{\mathrm{d}\psi}{\mathrm{d}t} = H\psi = g(S_x B_\perp \cos(\omega t) + S_y B_\perp \sin(\omega t) + S_z B)\psi.
\tag{22}
$$

The field is rotating in the same way as before. So, let's make the same substitution:

$$
\psi = U_z(\omega t)\psi'.
\tag{23}
$$

Here, $U_z(\omega t) = \exp(-i\omega t S_z/\hbar)$ is the rotation operator corresponding to the spin state space. Equation (22) then becomes

$$i\hbar\frac{\mathrm{d}U_z(\omega t)}{\mathrm{d}t}\psi' + i\hbar U_z(\omega t)\frac{\mathrm{d}\psi'}{\mathrm{d}t} = HU_z(\omega t)\psi' \tag{24}$$

and taking $U_z(-\omega t)$ on the left of both side yields

$$i\hbar\frac{\mathrm{d}\psi'}{\mathrm{d}t} = \left[U_z(-\omega t)HU_z(\omega t) - i\hbar U_z(-\omega t)\frac{\mathrm{d}U_z(\omega t)}{\mathrm{d}t}\right]\psi' \equiv H'\psi'. \tag{25}$$

Compare this with equation (11). Now, the new Hamiltonian H' is generally no easier to solve, but in the case of Rabi oscillation H' becomes constant (we've already checked using classical mechanics); this is because

$$
\begin{aligned}
U_z(-\omega t)HU_z(\omega t) &= g\vec{S}\cdot\left(R_z(-\omega t)\vec{B}\right) \\
&= g(S_x B_\perp + S_z B)
\end{aligned}
\tag{26}
$$

by the rotation theorem[2] and

$$
\begin{aligned}
U_z(-\omega t)\frac{\mathrm{d}U_z(\omega t)}{\mathrm{d}t} &= \exp\left(\frac{i\omega t S_z}{\hbar}\right)\frac{\mathrm{d}}{\mathrm{d}t}\exp\left(\frac{-i\omega t S_z}{\hbar}\right) \\
&= \exp\left(\frac{i\omega t S_z}{\hbar}\right)\left(\frac{-i\omega S_z}{\hbar}\right)\exp\left(\frac{-i\omega t S_z}{\hbar}\right) \\
&= \left(\frac{-i\omega S_z}{\hbar}\right)\exp\left(\frac{i\omega t S_z}{\hbar}\right)\exp\left(\frac{-i\omega t S_z}{\hbar}\right) \\
&= \frac{-i\omega S_z}{\hbar}.
\end{aligned}
\tag{27}
$$

Note that an alternative way to derive (26) and (27) is to adopt the standard basis of spin angular momentum operator for direct calculation.

$$S_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},\ S_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix},\ S_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{28}$$

Now, the Schrödinger equation for ψ' (25) simplifies to

$$
\begin{aligned}
i\hbar\frac{\mathrm{d}\psi'}{\mathrm{d}t} &= \left[S_x(gB_\perp) + S_z(gB - \omega)\right]\psi' \\
&\equiv \omega_p\left[S_x \sin\alpha + S_z \cos\alpha\right]\psi'
\end{aligned}
\tag{29}
$$

just as it was for the classical equation of motion. This solves to

$$\psi'(t) = \exp\left(\frac{-i\omega_p t\left[S_x \sin\alpha + S_z \cos\alpha\right]}{\hbar}\right)\psi'(0). \tag{30}$$

---

[2]This is not an official name. (I couldn't find one)

To simplify this, substitute $S_\mu = \hbar\sigma_\mu/2$ (σ_μ are the Pauli matrices) and use the extended Euler identity for Pauli matrices:

$$\exp(i\alpha\vec{\sigma}\cdot\hat{n}) = (\cos\alpha)I + (i\sin\alpha)\vec{\sigma}\cdot\hat{n}. \tag{31}$$

Then

$$\begin{aligned}
\psi'(t) &= \exp\left(\frac{-i\omega_p t}{2}[\sigma_x \sin\alpha + \sigma_z \cos\alpha]\right)\psi'(0)\\
&= \left[\cos\left(\frac{\omega_p t}{2}\right)I - i\sin\left(\frac{\omega_p t}{2}\right)[\sigma_x \sin\alpha + \sigma_z \cos\alpha]\right]\psi'(0)\\
&= U_y(\alpha)U_z(\omega_p t)U_y(-\alpha)\psi'(0).
\end{aligned} \tag{32}$$

Assuming the initial state to be $\psi'(0) = |\uparrow_z\rangle$, the above equation becomes

$$\psi'(t) = \cos\left(\frac{\omega_p t}{2}\right)|\uparrow_z\rangle - i\sin\left(\frac{\omega_p t}{2}\right)[\sin\alpha|\downarrow_z\rangle + \cos\alpha|\uparrow_z\rangle] \tag{33}$$

where we used $\sigma_x = |\uparrow_z\rangle\langle\downarrow_z| + |\downarrow_z\rangle\langle\uparrow_z|$ and $\sigma_z = |\uparrow_z\rangle\langle\uparrow_z| - |\downarrow_z\rangle\langle\downarrow_z|$. The probability of observing the down-spin state $|\downarrow_z\rangle$ is thus

$$\begin{aligned}
p_\downarrow(t) &= |\langle\downarrow_z|\psi\rangle|^2 = |\langle\downarrow_z|U_z(\omega t)\psi'\rangle|^2\\
&= |\langle\downarrow_z U_z^\dagger(\omega t)|\psi'\rangle|^2\\
&= |\langle\downarrow_z U_z(-\omega t)|\psi'\rangle|^2\\
&= |\langle\downarrow_z|\psi'\rangle|^2 \qquad (\because |\downarrow_z\rangle \text{ is parallel to the z-axis})\\
&= \left|-i\sin\left(\frac{\omega_p t}{2}\right)\sin\alpha\right|^2 = \sin^2\alpha \sin^2\left(\frac{\omega_p t}{2}\right)\\
&= \frac{(gB_\perp)^2}{(gB_\perp)^2 + (gB - \omega)^2}\sin^2\left(\frac{\sqrt{(gB_\perp)^2 + (gB - \omega)^2}}{2}t\right)
\end{aligned} \tag{34}$$

as we obtained for the classical case. Notice that the overall mathematical structure underlying our solution is exactly the same for classical mechanics and QM.

3.3 The rotating-wave approximation