Ph195a lecture notes, 11/21/01

The Bloch Equations

A quick review of spin-$\frac{1}{2}$ conventions and notation

The quantum state of a spin-$\frac{1}{2}$ particle is represented by a vector in a two-dimensional complex Hilbert space H_2.
Let $|+_z\rangle$ and $|-_z\rangle$ be eigenstates of the operator corresponding to component of spin along the z coordinate axis,

$$\mathbf{S}_z|+_z\rangle = +\frac{\hbar}{2}|+_z\rangle,$$
$$\mathbf{S}_z|-_z\rangle = -\frac{\hbar}{2}|-_z\rangle. \quad (1)$$

In this basis, the operators corresponding to spin components projected along the z, y, x coordinate axes may be represented by the following matrices:

$$\mathbf{S}_z = \frac{\hbar}{2}\boldsymbol{\sigma}_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$
$$\mathbf{S}_x = \frac{\hbar}{2}\boldsymbol{\sigma}_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$
$$\mathbf{S}_y = \frac{\hbar}{2}\boldsymbol{\sigma}_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}. \quad (2)$$

We commonly use $|\pm_x\rangle$ to denote eigenstates of $\mathbf{S}_x$, and similarly for $\mathbf{S}_y$. The dimensionless matrices $\boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y, \boldsymbol{\sigma}_z$ are known as the *Pauli matrices*, and satisfy the following commutation relations:

$$[\boldsymbol{\sigma}_x, \boldsymbol{\sigma}_y] = 2i\boldsymbol{\sigma}_z, \quad [\boldsymbol{\sigma}_y, \boldsymbol{\sigma}_z] = 2i\boldsymbol{\sigma}_x, \quad [\boldsymbol{\sigma}_z, \boldsymbol{\sigma}_x] = 2i\boldsymbol{\sigma}_y. \quad (3)$$

In addition,

$$\mathrm{Tr}[\boldsymbol{\sigma}_i\boldsymbol{\sigma}_j] = 2\delta_{ij}, \quad (4)$$

and

$$\boldsymbol{\sigma}_x^2 = \boldsymbol{\sigma}_y^2 = \boldsymbol{\sigma}_z^2 = \mathbf{1}. \quad (5)$$

The Pauli matrices are both Hermitian and unitary.

An arbitrary state for an isolated spin-$\frac{1}{2}$ particle may be written

$$|\Psi\rangle = \cos\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)|+_z\rangle + \sin\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)|-_z\rangle, \quad (6)$$

where θ and φ are real parameters that may be chosen in the ranges $0 \le \theta \le \pi$ and $0 \le \varphi \le 2\pi$. Note that there should really be four real degrees of freedom for a vector in a two-dimensional complex Hilbert space, but one is removed by normalization and another because we don't care about the overall phase of the state of an *isolated* quantum system.

Through the (θ, φ) representation, an arbitrary pure state may be represented as a point on the surface of a sphere, often referred to as the "Bloch Sphere," with θ as polar angle (latitude) and φ as azimuthal angle (longitude). The vector pointing from the original (center) of the Bloch Sphere to the point representing a quantum state is known as the Bloch vector corresponding to that state. The north and south poles thus correspond to $| +_z \rangle$ and $| -_z \rangle$, respectively, and

$$\begin{aligned} | +_x \rangle &\leftrightarrow \left(\theta = \frac{\pi}{2}, \varphi = 0\right), \quad | -_x \rangle \leftrightarrow \left(\theta = \frac{\pi}{2}, \varphi = \pi\right), \\ | +_y \rangle &\leftrightarrow \left(\theta = \frac{\pi}{2}, \varphi = \frac{\pi}{2}\right), \quad | -_y \rangle \leftrightarrow \left(\theta = \frac{\pi}{2}, \varphi = \frac{3\pi}{2}\right). \end{aligned} \qquad 7$$

With the sign conventions we have chosen, directions on the Bloch Sphere correspond to directions in coordinate space. Hence the state corresponding to spin pointing along a unit vector

$$\hat{u} = \begin{pmatrix} u_x & u_y & u_z \end{pmatrix} \qquad 8$$

(with $u_x^2 + u_y^2 + u_z^2 = 1$) has Bloch angles

$$\theta = \sin^{-1}\left(\sqrt{u_x^2 + u_y^2}\right), \quad \varphi = \tan^{-1}\left(\frac{u_y}{u_x}\right). \qquad 9$$

Likewise, the operator corresponding to component of spin along the $\hat{u}$-direction is

$$\begin{aligned} \mathbf{S}_u &= \vec{\mathbf{S}} \cdot \hat{u} = \sin\theta\cos\varphi\mathbf{S}_x + \sin\theta\sin\varphi\mathbf{S}_y + \cos\theta\mathbf{S}_z \\ &\leftrightarrow \frac{\hbar}{2}\begin{pmatrix} \cos\theta & \sin\theta\exp(-i\varphi) \\ \sin\theta\exp(i\varphi) & -\cos\theta \end{pmatrix}. \end{aligned} \qquad 10$$

The (θ, φ) representation defined above has the additional nice property that

$$
\begin{aligned}
\langle \mathbf{S}_x \rangle &= \frac{\hbar}{2}\left(\cos\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)\langle +_z | + \sin\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)\langle -_z |\right) \\
&\quad \times \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}\left(\cos\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)| +_z \rangle + \sin\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)| -_z \rangle\right) \\
&= \frac{\hbar}{2}\left(\cos\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)\langle +_z | + \sin\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)\langle -_z |\right) \\
&\quad \times \left(\cos\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)| -_z \rangle + \sin\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)| +_z \rangle\right) \\
&= \frac{\hbar}{2}\left(\cos\frac{\theta}{2}\sin\frac{\theta}{2}\exp(i\varphi) + \sin\frac{\theta}{2}\cos\frac{\theta}{2}\exp(-i\varphi)\right) \\
&= \frac{\hbar}{2}\sin\theta\cos\varphi, \\
\langle \mathbf{S}_y \rangle &= \frac{\hbar}{2}\left(\cos\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)\langle +_z | + \sin\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)\langle -_z |\right) \\
&\quad \times \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}\left(\cos\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)| +_z \rangle + \sin\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)| -_z \rangle\right) \\
&= \frac{\hbar}{2}\left(\cos\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)\langle +_z | + \sin\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)\langle -_z |\right) \\
&\quad \times \left(i\cos\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)| -_z \rangle - i\sin\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)| +_z \rangle\right) \\
&= \frac{\hbar}{2}\left(-i\cos\frac{\theta}{2}\sin\frac{\theta}{2}\exp(i\varphi) + i\sin\frac{\theta}{2}\cos\frac{\theta}{2}\exp(-i\varphi)\right) \\
&= \frac{\hbar}{2}\sin\theta\sin\varphi, \\
\langle \mathbf{S}_z \rangle &= \frac{\hbar}{2}\left(\cos\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)\langle +_z | + \sin\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)\langle -_z |\right) \\
&\quad \times \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}\left(\cos\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)| +_z \rangle + \sin\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)| -_z \rangle\right) \\
&= \frac{\hbar}{2}\left(\cos\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)\langle +_z | + \sin\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)\langle -_z |\right) \\
&\quad \times \left(\cos\frac{\theta}{2}\exp\left(-i\frac{\varphi}{2}\right)| +_z \rangle - \sin\frac{\theta}{2}\exp\left(i\frac{\varphi}{2}\right)| -_z \rangle\right) \\
&= \frac{\hbar}{2}\left(\cos^2\frac{\theta}{2} - \sin^2\frac{\theta}{2}\right) \\
&= \frac{\hbar}{2}\cos\theta.
\end{aligned} \tag{11}
$$

Hence we see that $\langle \vec{\mathbf{S}} \rangle \equiv \langle \mathbf{S}_x \rangle \hat{x} + \langle \mathbf{S}_y \rangle \bar{y} + \langle \mathbf{S}_z \rangle \hat{z}$, as a vector in coordinate space, coincides exactly with the Bloch vector.

It is important to remember that orthogonal states in H_2 are represented by ***antipodal*** points on the Bloch sphere – that is, points with angular separation π. In Hilbert space or in coordinate space, of course, orthogonal vectors have angular separation $\pi/2$. Hence the division by 2 in equation (6), which defines (θ, φ). The origin of this discrepancy has to do with the fact that the operators $\mathbf{S}_u$ correspond to a “spinor” representation of the $3D$ rotation group on a $2D$ complex vector space (more on this next term).

Dynamics on the Bloch Sphere – static fields

As long as we are concerned only with the spin degree of freedom for a spin-$\frac{1}{2}$ particle (ignoring particle motion), Hamiltonian dynamics depend only on the particle's gyromagnetic ratio γ and the applied magnetic field $\vec{B}$:

$$\begin{aligned}\mathbf{H} &= -\gamma\vec{\mathbf{S}}\cdot\vec{B}\\ &= -\gamma(\mathbf{S}_x B_x + \mathbf{S}_y B_y + \mathbf{S}_z B_z).\end{aligned} \quad 12$$

When $\vec{B}$ is static (time-independent), we are free to choose a coordinate system in which the z axis corresponds to the direction of $\vec{B}$. Then

$$\mathbf{H} = -\gamma\mathbf{S}_z B_z = \omega_L\mathbf{S}_z, \quad 13$$

where $\omega_L = -\gamma B_z$ is known as the Larmor frequency, and the energy eigenstates simply correspond to the $\mathbf{S}_z$ eigenstates,

$$\begin{aligned}\mathbf{H}|+_z\rangle &= \varepsilon_+|+_z\rangle, \quad \varepsilon_+ = +\frac{1}{2}\hbar\omega_L,\\ \mathbf{H}|-_z\rangle &= \varepsilon_-|-_z\rangle, \quad \varepsilon_- = -\frac{1}{2}\hbar\omega_L.\end{aligned} \quad 14$$

The time evolution of an arbitrary initial state

$$|\Psi(t=0)\rangle = \cos\frac{\theta_0}{2}\exp\left(-i\frac{\varphi_0}{2}\right)|+_z\rangle + \sin\frac{\theta_0}{2}\exp\left(i\frac{\varphi_0}{2}\right)|-_z\rangle, \quad 15$$

is thus given by

$$\begin{aligned}|\Psi(t)\rangle &= \cos\frac{\theta_0}{2}\exp\left(-i\frac{\varphi_0}{2}\right)\exp(-i\varepsilon_+t/\hbar)|+_z\rangle\\ &\quad + \sin\frac{\theta_0}{2}\exp\left(i\frac{\varphi_0}{2}\right)\exp(-i\varepsilon_-t/\hbar)|-_z\rangle,\\ &= \cos\frac{\theta_0}{2}\exp\left(-i\frac{\varphi(t)}{2}\right)|+_z\rangle + \sin\frac{\theta_0}{2}\exp\left(i\frac{\varphi(t)}{2}\right)|-_z\rangle,\end{aligned} \quad 16$$

where

$$\varphi(t) = \varphi_0 + \omega_L t. \quad 17$$

Hence, we find that the Bloch vector (from the center of the Bloch sphere to the point representing $|\Psi(t)\rangle$) simply precesses around the z axis with angular frequency ω_L.

To see this another way, we can write

$$\begin{aligned}\left\langle\vec{\mathbf{S}}\right\rangle &\equiv \langle\mathbf{S}_x\rangle\bar{x} + \langle\mathbf{S}_y\rangle\bar{y} + \langle\mathbf{S}_z\rangle\bar{z}\\ &= \frac{\hbar}{2}[\sin\theta_0\cos\varphi(t)\,\bar{x} + \sin\theta_0\sin\varphi(t)\,\bar{y} + \cos\theta_0\,\bar{z}],\end{aligned} \quad 18$$

which we may also use to denote that the instantaneous direction of the spin's precession corresponds to that of $\gamma\left\langle\vec{\mathbf{S}}\right\rangle\times\vec{B}$ (note that γ is negative for a bare electron, but may be either positive or negative for a composite spin-$\frac{1}{2}$ "particle" such as an atom or nucleus). In fact, we may write

$$\frac{d}{dt}\left\langle\vec{\mathbf{S}}\right\rangle = \gamma\left\langle\vec{\mathbf{S}}\right\rangle\times\vec{B}, \quad 19$$

in perfect agreement with the ***classical*** equations of motion for a magnetic moment in a static magnetic field!

Since this basic dynamical picture should be independent of the coordinate system we have chosen, we may conclude in general that the evolution of a spin-$\frac{1}{2}$ particle in an applied magnetic field $\vec{B}$ corresponds to "Larmor precession" of the spin around $\vec{B}$ with angular frequency $\omega_L = -\gamma\left|\vec{B}\right|$. Moreover, this precession should proceed precisely as predicted by the vector equation (19). Hence, if $|\Psi(0)\rangle = |-_z\rangle$ and $(B_x, B_y, B_z) = (B_0, 0, 0)$, we can guess that (assuming $\gamma < 0$)

$$|\Psi(t)\rangle = \sin(\omega_L t/2)|+_z\rangle + i\cos(\omega_L t/2)|-_z\rangle. \qquad 20$$

Here we have inferred the relative phase of $\exp(i\varphi) = i$ from the geometric picture that $|\Psi(t)\rangle$ should proceed from $|-_z\rangle$ to $|+_z\rangle$ through $|+_y\rangle$. We may compute explicitly,

$$\begin{aligned}
|\Psi(0)\rangle &= |-_z\rangle = \frac{1}{\sqrt{2}}[|+_x\rangle - |-_x\rangle],\\
|\Psi(t)\rangle &= \frac{1}{\sqrt{2}}[\exp(-i\omega_L t/2)|+_x\rangle - \exp(+i\omega_L t/2)|-_x\rangle]\\
&= \frac{1}{2}[\exp(-i\omega_L t/2)(|+_z\rangle + |-_z\rangle) - \exp(+i\omega_L t/2)(|+_z\rangle - |-_x\rangle)]\\
&= \frac{1}{2}[-2i\sin(\omega_L t/2)|+_z\rangle + 2\cos(\omega_L t/2)|-_z\rangle]\\
&= -i[\sin(\omega_L t/2)|+_z\rangle + i\cos(\omega_L t/2)|-_z\rangle],
\end{aligned} \qquad 21$$

which agrees with our prediction (20), up to overall phase.

The basic phenomenon of Larmor precession is quite useful in experiments where one needs to detect, *e.g.*, the presence of spin-$\frac{1}{2}$ particles in a given volume of space. One standard detection method is to apply a large magnetic field $\vec{B}$ perpendicular to the expected direction of $\left\langle\vec{\mathbf{S}}\right\rangle$. The spins will then precess at an appropriate Larmor frequency. Since the spins project a magnetic field pattern whose orientation is determined by $\left\langle\vec{\mathbf{S}}\right\rangle$, Larmor precession also implies a period modulation in the magnetic field flux through any plane containing $\vec{B}$. Using an inductive pickup coil, this periodic flux modulation can be detected via the induced EMF. According to Lenz's Law, this induced EMF should increase with the rate of change of the magnetic flux through the pickup coil, which in turn should increase with ω_L. Hence, large $\left|\vec{B}\right|$ translates into high sensitivity in such detection methods.

Note that in both of the Larmor precession examples above, $|\Psi(t)\rangle$ is only periodic in ω_L up to an overall minus sign. That is, when $t = 2\pi/|\omega_L|$, $|\Psi(t)\rangle = -|\Psi(0)\rangle$. This sign flip, which is sometimes known as the "spinor property" of spin-$\frac{1}{2}$ state vectors, is not just some artifact of our definitions of (θ, φ) on the Bloch Sphere – it is real, and can be observed in experiments. To see how this is possible, consider a composite system involving both a spin-$\frac{1}{2}$ particle and an auxilliary two-dimensional quantum system. We'll denote the spin-$\frac{1}{2}$ Hilbert space by H_A and the auxilliary Hilbert space by H_B. What we need is to arrange a situation where the overall Hamiltonian is given by

$$\mathbf{H}_{AB} = |1_B\rangle\langle 1_B| \otimes (-\gamma\mathbf{S}_z B_z), \qquad 22$$

where $\{|0_B\rangle, |1_B\rangle\}$ is an orthonormal basis for H_B and $\mathbf{S}_z$ acts on H_A only. This type of Hamiltonian could be realized, for example, if H_B corresponds to something like the position of the spin-$\frac{1}{2}$ particle being inside or outside of a region of applied magnetic field B_z. Then if the initial state

$$|\Psi_{AB}(0)\rangle = \frac{1}{\sqrt{2}}(|0_B\rangle + |1_B\rangle) \otimes |-_x\rangle$$
$$= \frac{1}{\sqrt{2}}(|0_B\rangle \otimes |-_x\rangle + |1_B\rangle \otimes |-_x\rangle) \qquad 23$$

is prepared, the state at a time $t = 2\pi/|\omega_L|$ later should be

$$|\Psi_{AB}(t)\rangle = \frac{1}{\sqrt{2}}(|0_B\rangle \otimes |-_x\rangle - |1_B\rangle \otimes |-_x\rangle)$$
$$= \frac{1}{\sqrt{2}}(|0_B\rangle - |1_B\rangle) \otimes |-_x\rangle. \qquad 24$$

Hence

$$\langle \Psi_{AB}(t)|\Psi_{AB}(0)\rangle = 0, \qquad 25$$

purely by virtue of the spinor property of the spin degree of freedom!

Before moving on to time-dependent magnetic fields, let us note the following fact. If we start out with a static applied field

$$\vec{B} = B_0\,\bar{z} \qquad 26$$

and a spin-$\frac{1}{2}$ particle prepared in the state $|+_z\rangle$ (or $|-_z\rangle$), there is no *finite* perturbation $\mathbf{W} = -\gamma\vec{\mathbf{S}} \cdot \vec{B}'$ (where $\vec{B}'$ lies in the $x-y$ plane) we can add to $H_0 = -\gamma\mathbf{S}_z B_0$ such that the particle will eventually evolve into the state $|-_z\rangle$ (or $|+_z\rangle$). Simply put, this is because for nonzero B_0 there is no finite $\vec{B}'$ such that $\vec{B}_{tot} = B_0\,\bar{z} + \vec{B}'$ is orthogonal to the z coordinate axis. Hence

$$\frac{d}{dt}\left\langle\vec{\mathbf{S}}\right\rangle = \gamma\left\langle\vec{\mathbf{S}}\right\rangle \times \vec{B}_{tot} \qquad 27$$

will never map $|+_z\rangle$ into $|-_z\rangle$ (or vice-versa).

Since one commonly utilizes large “holding fields” B_0 in order to achieve strong induction signals in spin-detection experiments (as described above), it would appear that more sophisticated control measures must be applied in order to do things like “flip” the spins in an experimental sample. This leads us now to time-dependent magnetic fields and the phenomenon of magnetic resonance.

Time-dependent magnetic fields

In the previous section we examined the phenomenon of Larmor precession, which for a static applied magnetic field $\vec{B} = B_0\,\bar{z}$ leads to state evolutions of the form

$$|\Psi(t)\rangle = \cos\frac{\theta_0}{2}\exp\left(-i\frac{\varphi(t)}{2}\right)|+_z\rangle + \sin\frac{\theta_0}{2}\exp\left(i\frac{\varphi(t)}{2}\right)|-_z\rangle \qquad 28$$

with $\varphi(t) = \varphi_0 + \omega_L t = \varphi_0 - \gamma B_0 t.$ Formally, this state evolution corresponds to Hamiltonian evolution that can also be described as the effect of a unitary time-development operator:

$$|\Psi(t)\rangle = \exp(-i\mathbf{H}_0\,t/\hbar)|\Psi(0)\rangle$$
$$= \exp(-i\omega_L\boldsymbol{\sigma}_z\,t/2)|\Psi(0)\rangle. \qquad 29$$

In what follows we shall assume the existence of a fixed holding field $\vec{B} = B_0\,\bar{z}$ at all times.

Accordingly, it will be convenient to work in a "rotating frame" that *formally* eliminates the constant Larmor precession. Although it may not be obvious that this is worth the trouble, it is.

Geometrically, we can think of defining time-dependent coordinate axes

$$\begin{aligned} \bar{x}'(t) &= \bar{x}\cos(\omega t) + \bar{y}\sin(\omega t), \\ \bar{y}'(t) &= -\bar{x}\sin(\omega t) + \bar{y}\cos(\omega t), \\ \bar{z}'(t) &= \bar{z}, \end{aligned} \tag{30}$$

such that if we set $\omega = \omega_L$ we may expect

$$\begin{aligned} \left\langle \vec{\mathbf{S}} \right\rangle \cdot \bar{x}'(t) &= \frac{\hbar}{2}(\sin\theta\cos\varphi(t)\cos(\omega_L t) + \sin\theta\sin\varphi(t)\sin(\omega_L t)), \\ \left\langle \vec{\mathbf{S}} \right\rangle \cdot \bar{y}'(t) &= \frac{\hbar}{2}(-\sin\theta\cos\varphi(t)\sin(\omega_L t) + \sin\theta\sin\varphi(t)\cos(\omega_L t)), \\ \left\langle \vec{\mathbf{S}} \right\rangle \cdot \bar{z}'(t) &= \frac{\hbar}{2}\cos\theta, \end{aligned} \tag{31}$$

all to be constant. Indeed, since

$$\begin{aligned} \cos\varphi(t) &= \cos(\varphi_0 + \omega_L t) = \cos\varphi_0\cos\omega_L t - \sin\varphi_0\sin\omega_L t, \\ \sin\varphi(t) &= \sin(\varphi_0 + \omega_L t) = \sin\varphi_0\cos\omega_L t + \cos\varphi_0\sin\omega_L t, \end{aligned} \tag{32}$$

we have

$$\begin{aligned} \left\langle \vec{\mathbf{S}} \right\rangle \cdot \bar{x}'(t) &= \frac{\hbar}{2}\sin\theta(\cos\varphi_0\cos\omega_L t - \sin\varphi_0\sin\omega_L t)\cos(\omega_L t) \\ &\quad + \frac{\hbar}{2}\sin\theta(\sin\varphi_0\cos\omega_L t + \cos\varphi_0\sin\omega_L t)\sin(\omega_L t) \\ &= \frac{\hbar}{2}\sin\theta\cos\varphi_0, \\ \left\langle \vec{\mathbf{S}} \right\rangle \cdot \bar{y}'(t) &= -\frac{\hbar}{2}\sin\theta(\cos\varphi_0\cos\omega_L t - \sin\varphi_0\sin\omega_L t)\sin(\omega_L t) \\ &\quad + \frac{\hbar}{2}\sin\theta(\sin\varphi_0\cos\omega_L t + \cos\varphi_0\sin\omega_L t)\cos(\omega_L t) \\ &= \frac{\hbar}{2}\sin\theta\sin\varphi_0. \end{aligned} \tag{33}$$

In terms of the quantum state vector, however, it would appear that we should define

$$\begin{aligned} |\Psi'(t)\rangle &= \exp(+i\omega_L \boldsymbol{\sigma}_z t/2)|\Psi(t)\rangle \\ &\equiv \mathbf{O}_z|\Psi(t)\rangle \end{aligned} \tag{34}$$

(here we are defining the unitary operator $\mathbf{O}_z$). Then $|\Psi'(t)\rangle = |\Psi'(0)\rangle$ as long as the Hamiltonian is given simply by

$$\mathbf{H}_0 = \omega_L \mathbf{S}_z. \tag{35}$$

However, in order to continue using $|\Psi'(t)\rangle$ in the presence of perturbations, we need to derive its general equation of motion in the rotating frame. Let us also return to a general setting in which the frequency ω that defines the rotating frame via

$$\begin{aligned} |\Psi'(t)\rangle &= \mathbf{O}_z|\Psi(t)\rangle \\ &= \exp(+i\omega\boldsymbol{\sigma}_z t/2)|\Psi(t)\rangle \end{aligned} \tag{36}$$

is independent of ω_L. We can start from the Schrödinger Equation

$$\begin{aligned} i\hbar\frac{d}{dt}|\Psi(t)\rangle &= \mathbf{H}|\Psi(t)\rangle \\ &= \mathbf{H}\mathbf{O}_z^{-1}|\Psi'(t)\rangle. \end{aligned} \tag{37}$$

On the left-hand side, we may also apply the chain rule to yield

$$\begin{aligned} i\hbar\frac{d}{dt}|\Psi(t)\rangle &= i\hbar\frac{d}{dt}\left(\mathbf{O}_z^{-1}|\Psi'(t)\rangle\right) \\ &= i\hbar\left(\frac{d\mathbf{O}_z^{-1}}{dt}|\Psi'(t)\rangle + \mathbf{O}_z^{-1}\frac{d}{dt}|\Psi'(t)\rangle\right). \end{aligned} \qquad 38$$

Hence, combining the two expressions and multiplying through from the left by $\mathbf{O}_z$, we obtain

$$\begin{aligned} i\hbar\frac{d}{dt}|\Psi'(t)\rangle &= \left(\mathbf{O}_z\mathbf{H}\mathbf{O}_z^{-1} - i\hbar\mathbf{O}_z\frac{d\mathbf{O}_z^{-1}}{dt}\right)|\Psi'(t)\rangle \\ &\equiv \mathbf{H}'|\Psi'(t)\rangle. \end{aligned} \qquad 39$$

Recall that since $\mathbf{O}_z$ is unitary, $\mathbf{O}_z^{-1} = \mathbf{O}_z^{\dagger}$. Hence

$$\begin{aligned} -i\hbar\mathbf{O}_z\frac{d\mathbf{O}_z^{-1}}{dt} &= -i\hbar\exp(+i\omega\boldsymbol{\sigma}_z t/2)\frac{d}{dt}\exp(-i\omega\boldsymbol{\sigma}_z t/2) \\ &= -i\hbar\exp(+i\omega\boldsymbol{\sigma}_z t/2)\frac{d}{dt}\sum_{n=0}^{\infty}\frac{1}{n!}(-i\omega\boldsymbol{\sigma}_z t/2)^n \\ &= -i\hbar\exp(+i\omega\boldsymbol{\sigma}_z t/2)\sum_{n=1}^{\infty}\frac{n}{n!}(-i\omega\boldsymbol{\sigma}_z t/2)^{n-1}(-i\omega\boldsymbol{\sigma}_z/2) \\ &= -i\hbar\exp(+i\omega\boldsymbol{\sigma}_z t/2) \\ &\quad\times\sum_{n=1}^{\infty}\frac{1}{(n-1)!}(-i\omega\boldsymbol{\sigma}_z t/2)^{n-1}(-i\omega\boldsymbol{\sigma}_z/2) \\ &= -i\hbar\exp(+i\omega\boldsymbol{\sigma}_z t/2)\exp(-i\omega\boldsymbol{\sigma}_z t/2)(-i\omega\boldsymbol{\sigma}_z/2) \\ &= \frac{-\hbar\omega}{2}\boldsymbol{\sigma}_z. \end{aligned} \qquad 40$$

Now we can finally make use of all this to solve for the effects of a time-dependent perturbation,

$$\begin{aligned} \mathbf{W}(t) &= -\gamma b_1(\bar{x}\cos(\omega t) + \bar{y}\sin(\omega t))\cdot\vec{\mathbf{S}} \\ &= -\gamma b_1\frac{\hbar}{2}(\cos(\omega t)\boldsymbol{\sigma}_x + \sin(\omega t)\boldsymbol{\sigma}_y). \end{aligned} \qquad 41$$

Here b_1 is a magnetic field strength. At this point it is convenient to define new operators

$$\begin{aligned} \boldsymbol{\sigma}_+ &= \frac{1}{2}(\boldsymbol{\sigma}_x + i\boldsymbol{\sigma}_y), \\ \boldsymbol{\sigma}_- &= \frac{1}{2}(\boldsymbol{\sigma}_x - i\boldsymbol{\sigma}_y), \end{aligned} \qquad 42$$

in terms of which

$$\mathbf{W}(t) = -\gamma b_1\frac{\hbar}{2}(\exp(-i\omega t)\boldsymbol{\sigma}_+ + \exp(+i\omega t)\boldsymbol{\sigma}_-). \qquad 43$$

Noting the commutation relations

$$\begin{aligned}
[\boldsymbol{\sigma}_+,\boldsymbol{\sigma}_z] &= \frac{1}{2}([\boldsymbol{\sigma}_x,\boldsymbol{\sigma}_z] + i[\boldsymbol{\sigma}_y,\boldsymbol{\sigma}_z]) \\
&= \frac{1}{2}(-2i\boldsymbol{\sigma}_y - 2\boldsymbol{\sigma}_x) \\
&= -2\boldsymbol{\sigma}_+, \\
[\boldsymbol{\sigma}_-,\boldsymbol{\sigma}_z] &= \frac{1}{2}([\boldsymbol{\sigma}_x,\boldsymbol{\sigma}_z] - i[\boldsymbol{\sigma}_y,\boldsymbol{\sigma}_z]) \\
&= \frac{1}{2}(-2i\boldsymbol{\sigma}_y + 2\boldsymbol{\sigma}_x) \\
&= 2\boldsymbol{\sigma}_-,
\end{aligned} \tag{44}$$

we have

$$\begin{aligned}
\mathbf{H}' &= \mathbf{O}_z\mathbf{H}\mathbf{O}_z^{-1} - i\hbar\mathbf{O}_z\frac{d\mathbf{O}_z^{-1}}{dt} \\
&= \mathbf{O}_z(\mathbf{H}_0 + \mathbf{W})\mathbf{O}_z^{-1} - \frac{\hbar\omega}{2}\boldsymbol{\sigma}_z \\
&= \mathbf{O}_z\left(\frac{\hbar\omega_L}{2}\boldsymbol{\sigma}_z - \gamma b_1\frac{\hbar}{2}(\exp(-i\omega t)\boldsymbol{\sigma}_+ + \exp(+i\omega t)\boldsymbol{\sigma}_-)\right)\mathbf{O}_z^{-1} - \frac{\hbar\omega}{2}\boldsymbol{\sigma}_z \\
&= \frac{1}{2}\hbar\Delta\boldsymbol{\sigma}_z - \gamma b_1\frac{\hbar}{2}\exp(+i\omega\boldsymbol{\sigma}_z t/2) \\
&\quad \times (\exp(-i\omega t)\boldsymbol{\sigma}_+ + \exp(+i\omega t)\boldsymbol{\sigma}_-)\exp(-i\omega\boldsymbol{\sigma}_z t/2),
\end{aligned} \tag{45}$$

where $\Delta \equiv \omega_L - \omega$ and we have used the fact that $\left[\boldsymbol{\sigma}_z, \mathbf{O}_z^{-1}\right] = [\boldsymbol{\sigma}_z, \exp(-i\omega\boldsymbol{\sigma}_z t/2)] = 0$. Next we need to compute

$$\begin{aligned}
\boldsymbol{\sigma}_+\exp(-i\omega\boldsymbol{\sigma}_z t/2) &= \boldsymbol{\sigma}_+\sum_{n=0}^{\infty}\frac{1}{n!}(-i\omega\boldsymbol{\sigma}_z t/2)^n \\
&= \sum_{n=0}^{\infty}\frac{1}{n!}(-i\omega t/2)^n(\boldsymbol{\sigma}_+\boldsymbol{\sigma}_z^n) \\
&= \sum_{n=0}^{\infty}\frac{1}{n!}(-i\omega t/2)^n(-1)^n\boldsymbol{\sigma}_+ \\
&= \exp(+i\omega t/2)\boldsymbol{\sigma}_+,
\end{aligned} \tag{46}$$

where in going from the second to the third line we have used the fact that

$$\begin{aligned}
\boldsymbol{\sigma}_+\boldsymbol{\sigma}_z &= \frac{1}{2}(\boldsymbol{\sigma}_x + i\boldsymbol{\sigma}_y)\boldsymbol{\sigma}_z \\
&= \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \\
&= \begin{pmatrix} 0 & -1 \\ 0 & 0 \end{pmatrix} \\
&= -\boldsymbol{\sigma}_+.
\end{aligned} \tag{47}$$

Similarly,

$$\begin{aligned}
\exp(+i\omega\boldsymbol{\sigma}_z t/2)\boldsymbol{\sigma}_+ &= \exp(+i\omega t/2)\boldsymbol{\sigma}_+, \\
\boldsymbol{\sigma}_-\exp(-i\omega\boldsymbol{\sigma}_z t/2) &= \exp(-i\omega t/2)\boldsymbol{\sigma}_-, \\
\exp(-i\omega\boldsymbol{\sigma}_z t/2)\boldsymbol{\sigma}_- &= \exp(+i\omega t/2)\boldsymbol{\sigma}_-,
\end{aligned} \tag{48}$$

and we finally arrive at

$$\begin{aligned}\mathbf{H}' &= \frac{1}{2}\hbar\Delta\boldsymbol{\sigma}_z - \gamma b_1 \frac{\hbar}{2}(\boldsymbol{\sigma}_+ + \boldsymbol{\sigma}_-) \\ &= \frac{1}{2}\hbar(\Delta\boldsymbol{\sigma}_z - \gamma b_1 \boldsymbol{\sigma}_x) \\ &= -\gamma\vec{\mathbf{S}} \cdot \vec{B}_{eff}, \end{aligned} \qquad 49$$

where

$$\vec{B}_{eff} = \left(B_0 + \frac{\omega}{\gamma}\right)\bar{z} + b_1\bar{x}. \qquad 50$$

Recall that $\omega_L = -\gamma B_0$, so if $\omega = \omega_L$ the z component of $\vec{B}_{eff}$ vanishes. And in general, we have the simple result that if $\Delta \ll \omega_L$, the magnitude of the effective holding field is greatly ***reduced*** in the rotating frame.

In particular, if $\Delta = 0$ then the Bloch vector corresponding to $|\Psi'(t)\rangle$ should simply precess around a static field $b_1\bar{x}'$ in the rotating frame. It thus follows that for an initial state such as $|\Psi(0)\rangle = |-_z\rangle$, the application of a rotating field

$$\vec{B}_\perp(t) = b_1(\bar{x}\cos(\omega_L t) + \bar{y}\sin(\omega_L t)) \qquad 51$$

will lead to $|\Psi(t)\rangle = |+_z\rangle$ at time $t = 2\pi/|\gamma b_1|$. This technique enables “perfect” spin flips even in the presence of a large holding field $B_0\bar{z}$.

Note however that if $\Delta \neq 0$, it is still impossible to achieve $|+_z\rangle \mapsto |-_z\rangle$ with finite b_1. Hence it is crucial to apply the rotating field $\vec{B}_\perp(t)$ exactly at the resonance frequency ω_L. As long as this condition is met, $|+_z\rangle \mapsto |-_z\rangle$ will happen eventually, even for very small b_1 (as long as we ignore dissipation!). In this sense we find that the frequency of the applied perturbation is much more important than its magnitude, at least for the purpose of perfectly flipping spins. This is generally referred to as the phenomenon of magnetic (or two-level) resonance.

Dynamics in the rotating frame

Having derived the form of the effective Hamiltonian

$$\mathbf{H}' = \frac{1}{2}\hbar(\Delta\boldsymbol{\sigma}_z - \gamma b_1 \boldsymbol{\sigma}_x) \qquad 52$$

in the rotating frame, we are able to apply our earlier results about the general behavior of two-level systems under static perturbations. We may define

$$\mathbf{H}_0' = \frac{1}{2}\hbar\Delta\boldsymbol{\sigma}_z, \quad \mathbf{W}' = -\frac{1}{2}\hbar\gamma b_1\boldsymbol{\sigma}_x, \qquad 53$$

as well as

$$\begin{aligned}\mathbf{H}_0'\left|\varphi_1'\right\rangle &= E_1|\varphi_1'\rangle, \quad E_1 = +\frac{1}{2}\hbar\Delta, \\ \mathbf{H}_0'\left|\varphi_2'\right\rangle &= E_2|\varphi_2'\rangle, \quad E_2 = -\frac{1}{2}\hbar\Delta,\end{aligned} \qquad 54$$

where

$$|\varphi_1'\rangle \leftrightarrow |+_z\rangle, \quad |\varphi_2'\rangle \leftrightarrow |-_z\rangle. \qquad 55$$

Then, *e.g.*, the eigenvalues of $\mathbf{H}'$ are given by

$$E_\pm = \frac{1}{2}(E_1 + W_{11} + E_2 + W_{22}) \pm \frac{1}{2}\sqrt{(E_1 + W_{11} - E_2 - W_{22})^2 + 4|W_{12}|^2}. \quad 56$$

With these exact expressions for the energy eigenvalues and eigenvectors, it is straightforward to compute the time-evolution of an arbitrary initial state *in the rotating frame*. We just have to be careful to transform back to the static (laboratory) frame at the end of the calculation, via

$$|\Psi(t)\rangle = \mathbf{O}_z^{-1}|\Psi'(t)\rangle. \quad 57$$