A Gentle Introduction to Spintronics

JEREMY LIAN

Division of Physics & Applied Physics
School of Physical & Mathematical Sciences
Nanyang Technological University

May 2020

Attention

This set of notes is meant to serve as a journal for my self-directed learning in the specified subject area, and also as a self-contained reference material for which I can document all important concepts from related sub-fields of physics. I have modified (often significantly) contents from course notes and literature resources in an effort to contextualise these information for the present subject matter, during which any such allusions made will be documented. They are nowhere near accurate representations of what was originally presented, and I can only hope for a passable – if not equal – standard of clarity in my presentation. Finally, all errors in this set of notes are almost certainly mine.

Contents

1 Spin-*ing* in Quantum Mechanics

In quantum mechanics, any physical observable is associated with an operator (linear operator in Schrödinger formalism, matrix in Heisenberg formalism). The eigenvalues of these operators are the expectation values of the physical quantity. Spin is a physical observable since the associated angular momentum can be measured (i.e., Stern-Gerlach experiment). Its origin lies in relativistic quantum mechanics and can be appreciated by the Dirac equation (which will be derived in sections). Consequently, there must be a quantum mechanical operator associated with spin.

1.1 Pauli Matrices in Spin Operators

Pauli's approach to derive the spin operators was based on the premise that:

1. electron spin angular momentum component along any coordinate axis should give the results $+\frac{\hbar}{2}$ or $-\frac{\hbar}{2}$
2. operators for spin components along the three orthogonal axes should obey commutation rules similar to those of the orbital angular momentum operators [1]

Thus, he defined for the spin operator components:

$$S_x = \frac{\hbar}{2}\sigma_x \tag{1}$$

$$S_y = \frac{\hbar}{2}\sigma_y \tag{2}$$

$$S_z = \frac{\hbar}{2}\sigma_z \tag{3}$$

where σ_x, σ_y, and σ_z are the Pauli matrices having the values:

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \tag{4}$$

$$\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \tag{5}$$

$$\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{6}$$

It is no coincidence that the square of the spin operator

$$[S]^2 = S_x^2 + S_y^2 + S_z^2 = \bar{s}(\bar{s}+1)\hbar^2[I] \tag{7}$$

(where $\bar{s} = \frac{1}{2}$) is analogously equivalent to the relation for the orbital angular momentum operator

$$[L]^2 = m(m+1)\hbar^2[I], \;\; m = 1, 2, 3, \cdots \tag{8}$$

Pauli had intended to put spin angular momentum and orbital angular momentum on the same footing.

1.1.1 Spinors as eigenvectors

We then require the Pauli matrix σ_z to satisfy the following eigenvalue equation:

$$\sigma_z \left|\pm\right\rangle_z = \pm 1 \left|\pm\right\rangle_z \tag{9}$$

Thus, these eigenvectors (with unit norm) will take on the values

$$\left|+\right\rangle_z = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \tag{10}$$

$$\left|-\right\rangle_z = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \tag{11}$$

It is easy to verify (through the inner product) that these two eigenvectors are orthonormal, as they must be since they are eigenvectors of a Hermitian matrix corresponding to distinct eigenvalues.

Likewise, both σ_x and σ_y satisfy similar eigenvalue equations, and their respective eigenvectors can be easily determined to be

$$|+\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \tag{12}$$

$$|-\rangle_x = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \tag{13}$$

$$|+\rangle_y = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix} \tag{14}$$

$$|-\rangle_y = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix} \tag{15}$$

It is easy to check that these eigenvectors can also be expressed as

$$|\pm\rangle_x = \frac{1}{\sqrt{2}}[|+\rangle_z \pm |-\rangle_z] \tag{16}$$

$$|\pm\rangle_y = \frac{1}{\sqrt{2}}[|+\rangle_z \pm i\,|-\rangle_z] \tag{17}$$

These eigenvectors are also called "spinors" which represent the spin state of an electron. If we know the spinor associated with an electron in a given state, we can deduce the electron's spin orientation, i.e., $\langle S\rangle$.

1.2 From Schrödinger to Pauli Equation

Let us declare for the (normalised) spinor wavefunction to have two components, i.e.,

$$[\psi(\mathbf{X})] = \begin{bmatrix}\phi_1(\mathbf{X})\\\phi_2(\mathbf{X})\end{bmatrix} \tag{18}$$

where $X \equiv (t, x, y, z)$.

The Schrödinger equation can then be recast as

$$\left\{[H] - i\hbar\frac{\partial}{\partial t}[I]\right\}[\psi(\mathbf{X})] = [0] \tag{19}$$

where the Hamiltonian is a $2 * 2$ matrix, $[I]$ is the $2 * 2$ identity matrix, and $[0]$ is the $2 * 1$ null vector. This is also known as the Pauli equation; a set of two simultaneous differential equations for the two components of the spinor wavefunction.

Solution of the Pauli equation yields the two-component spinor wavefunction $[\psi(\mathbf{X})]$, which will allow us to determine the three components of an electron's spin according to the following Dirac notations:

$$\begin{aligned}
\langle S_x\rangle(\mathbf{X}) &= [\psi(\mathbf{X})]^\dagger S_x[\psi(\mathbf{X})] && (20)\\
&= \frac{\hbar}{2}\begin{bmatrix}\phi_1^*(\mathbf{X}) & \phi_2^*(\mathbf{X})\end{bmatrix}\sigma_x\begin{bmatrix}\phi_1(\mathbf{X})\\\phi_2(\mathbf{X})\end{bmatrix} && (21)\\
&= \frac{\hbar}{2}\begin{bmatrix}\phi_1^*(\mathbf{X}) & \phi_2^*(\mathbf{X})\end{bmatrix}\begin{bmatrix}0 & 1\\1 & 0\end{bmatrix}\begin{bmatrix}\phi_1(\mathbf{X})\\\phi_2(\mathbf{X})\end{bmatrix} && (22)\\
&= \hbar\,\mathrm{Re}[\phi_1^*(\mathbf{X})\phi_2(\mathbf{X})] && (23)\\
\langle S_y\rangle(\mathbf{X}) &= \hbar\,\mathrm{Im}[\phi_1^*(\mathbf{X})\phi_2(\mathbf{X})] && (24)\\
\langle S_z\rangle(\mathbf{X}) &= \frac{\hbar}{2}\left[|\phi_1(\mathbf{X})|^2 - |\phi_2(\mathbf{X})|^2\right] && (25)
\end{aligned}$$

where Re stands for the real part, Im stands for the imaginary part, the superscript $*$ represents the complex conjugate, and the superscript $\dagger$ represents the Hermitian conjugate.

1.2.1 The Schrödinger-Pauli Hamiltonian

The Hamiltonian in Eq.19 is composed of three terms:

$$[H] = H_0[I] + [H_B] + [H_{SO}] \tag{26}$$

where H_0 is the spin-independent Hamiltonian.

$[H_B]$ gives the energy of the interaction between the self magnetic moment $\vec{\mu_{\mathbf{e}}}$ of the electron and an externally applied magnetic field $\vec{\mathbf{B}}$. This energy is given to be:

$$E_{\text{int}} = -\vec{\mu_{\mathbf{e}}} \cdot \vec{\mathbf{B}} \tag{27}$$

It is known that the ratio of the magnetic moment $\vec{\mu_{\mathbf{e}}}$ (in units of the Bohr magneton μ_B) to the spin angular momentum $\vec{\mathbf{S}}$ (in units of $\hbar$) is the so-called Landé g-factor g [2]. Therefore, the Hamiltonian associated with E_{int} is

$$[H_B] = \frac{g}{2}\mu_B \vec{\mathbf{B}} \cdot \vec{\sigma} \tag{28}$$

since $\vec{\mathbf{S}} = \frac{\hbar}{2}\vec{\sigma}$, where $\vec{\sigma} = \sigma_x\hat{\mathbf{x}} + \sigma_y\hat{\mathbf{y}} + \sigma_z\hat{\mathbf{z}}$.

It should be easy to see that the eigenenergies associated with this Hamiltonian will be distinct. Therefore, the degeneracy between the two spin states is lifted and this is given the name Zeeman splitting. The Hamiltonian $[H_B]$ is hence called the Zeeman interaction term. The Hamiltonian $[H_SO]$ is associated with spin-orbit interaction which also lifts the spin degeneracy. This interaction is further discussed in a later chapter.

1.3 Dirac - the Impossible Genius

A free electron not subjected to any forces has a constant potential energy which can be taken to be zero (since potential is always undefined to the extent of an arbitrary constant). According to Einstein's special theory of relativity, such an electron obeys the relation

$$E^2 = p^2c^2 + m_0^2c^4 \tag{29}$$

where E is the total energy, p is the momentum, c is the speed of light in vacuum space, and m_0 is the rest mass of the electron.

De Broglie postulated that,

$$E = hf \tag{30}$$

$$p = \frac{h}{\lambda} \tag{31}$$

where f is the frequency and λ is the De Broglie wavelength associated with the electron. Thus, Eq.29 can be re-written as

$$f^2 - \left(\frac{c}{\lambda}\right)^2 = \left(\frac{m_0c^2}{h}\right)^2 \tag{32}$$

We can write the quantum mechanical analogue of Eq.29 by promoting the physical quantities E and p into operators $i\hbar\frac{\partial}{\partial t}$ and $-i\hbar\frac{\partial}{\partial x_r}$ respectively. Therefore, the quantum mechanical representation of Eq.29 is

$$\left[\left(\frac{i\hbar}{c}\frac{\partial}{\partial t}\right)^2 - \sum_{r=1}^{3}\left(-i\hbar\frac{\partial}{\partial x_r}\right)^2 - m_0^2c^2\right]\psi(\mathbf{X}) = 0 \tag{33}$$

The above equation has the solution of a plane wave:

$$\psi(\mathbf{X}) = \psi(t, \vec{\mathbf{r}}) \tag{34}$$

$$= e^{i(\vec{\mathbf{k}}\cdot\vec{\mathbf{r}} - \omega t)} \tag{35}$$

where $\vec{\mathbf{k}} = \frac{2\pi}{\lambda}$, $\vec{\mathbf{r}} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}$, and $\omega = 2\pi f$.

It should be obvious that substituting this solution into Eq.33 immediately yields Eq.32.

Eq.33 is also known as the Klein-Gordon equation. However, Dirac in his transformation theory, had established the ground that all meaningful equations of quantum mechanics must be first order with respect to time (just like the Schrödinger and Pauli equations). Thus, in a stroke of genius, he proposed an alternative [3]:

$$\left[\left(\frac{i\hbar}{c}\frac{\partial}{\partial t}\right) - \sum_{r=1}^{3}\gamma_r\left(-i\hbar\frac{\partial}{\partial x_r}\right) - \gamma_0 m_0 c\right]\psi(\mathbf{X}) = 0 \tag{36}$$

which is now the famous Dirac equation. $\gamma_{0,1,2,3}$ are the Dirac matrices given by the values:

$$\gamma_0 = \begin{pmatrix} \mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \end{pmatrix} \tag{37}$$

$$\gamma_1 = \begin{pmatrix} \mathbf{0} & \sigma_1 \\ \sigma_1 & \mathbf{0} \end{pmatrix} \tag{38}$$

$$\gamma_2 = \begin{pmatrix} \mathbf{0} & \sigma_2 \\ \sigma_2 & \mathbf{0} \end{pmatrix} \tag{39}$$

$$\gamma_3 = \begin{pmatrix} \mathbf{0} & \sigma_3 \\ \sigma_3 & \mathbf{0} \end{pmatrix} \tag{40}$$

where $\mathbf{I}$ is a 2×2 identity matrix and $\mathbf{0}$ is a 2×2 null matrix.

The proof of theory can be done by calculating the atomic level spacings for a Hydrogen atom. More importantly, we can demonstrate that the orbital angular momentum alone is not a conserved quantity, but when the quantity represented by the spin operator

$$\frac{1}{2}\begin{pmatrix} \mathbf{0} & \sigma \\ \sigma & \mathbf{0} \end{pmatrix} \tag{41}$$

is added to it, the total quantity is conserved. Viewed from the perspective of conservation of total angular momentum, this shows that an electron has spin angular momentum given by the operator in Eq.41. This is the first convincing theoretical demonstration of the existence of spin and hence Dirac is credited with establishing the concept of spin rigorously. In the process, he also demonstrated that spin angular momentum must be quantized to two distinct values since the matrix in Eq.41 has two distinct and discrete eigenvalues. Therefore, Dirac was able to explain spin quantization, which the self rotation model of the electron could never explain by itself.

1.4 Further Discussions on Dirac Equation

Eq.36 is valid for a free electron. For an electron subjected to a (time-dependent) force field, let the time-dependent electromagnetic four-vector potential associated with the force field be $\mathbf{A} = (A_0, A_x, A_y, A_z)$. The Dirac equation in Eq.36 can then be modified as [4]

$$\left[\left(\frac{i\hbar}{c}\frac{\partial}{\partial t} + eA_0\right) - \sum_{r=1}^{3}\gamma_r\left(-i\hbar\frac{\partial}{\partial x_r} + eA_r\right) - \gamma_0 m_0 c\right]\psi(\mathbf{X}) = 0 \tag{42}$$

From the above, we can write the time *independent* Dirac equation (TIDE):

$$\begin{pmatrix} a & 0 & c & d^* \\ 0 & a & d & -c \\ c & d^* & b & 0 \\ d & -c & 0 & b \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} = E\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} \tag{43}$$

where we have denoted

$$a = m_0c^2 + V \tag{44}$$

$$b = -m_0c^2 + V \tag{45}$$

$$c = c(p_z + eA_z) \tag{46}$$

$$d = c[(p_x + eA_x) + i(p_y + eA_y)] \tag{47}$$

where $V = ecA_0$ is the typical scalar potential energy.

We can write this more compactly as

$$\begin{bmatrix} (m_0c^2 + V)[I] & c\vec{\sigma} \cdot [\vec{\mathbf{p}} + e\vec{\mathbf{A}}] \\ c\vec{\sigma} \cdot [\vec{\mathbf{p}} + e\vec{\mathbf{A}}] & (-m_0c^2 + V)[I] \end{bmatrix} \begin{bmatrix} \psi(x,y,z) \\ \phi(x,y,z) \end{bmatrix} = E \begin{bmatrix} \Psi(x,y,z) \\ \phi(x,y,z) \end{bmatrix} \tag{48}$$

where

$$\Psi(x,y,z) = \begin{bmatrix} \psi_1(x,y,z) \\ \psi_2(x,y,z) \end{bmatrix} \tag{49}$$

$$\phi(x,y,z) = \begin{bmatrix} \psi_3(x,y,z) \\ \psi_4(x,y,z) \end{bmatrix} \tag{50}$$

From here, we can show that

$$\left\{ (m_0c^2 + V)[I] + [c\vec{\sigma} \cdot (\vec{\mathbf{p}} + e\vec{\mathbf{A}})] \frac{1}{E + m_0c^2 - V} [I][c\vec{\sigma} \cdot (\vec{\mathbf{p}} + e\vec{\mathbf{A}})] \right\} \Psi = E\Psi \tag{51}$$

$$\left\{ (-m_0c^2 + V)[I] + [c\vec{\sigma} \cdot (\vec{\mathbf{p}} + e\vec{\mathbf{A}})] \frac{1}{E - m_0c^2 - V} [I][c\vec{\sigma} \cdot (\vec{\mathbf{p}} + e\vec{\mathbf{A}})] \right\} \phi = E\phi \tag{52}$$

1.4.1 Non-Relativistic Approximation

Consider a non-relativistic electron moving at speed $v \ll c$. Eq.29 yields $E \approx m_0c^2$. Using the first of the two equations above yields

$$\left\{ (m_0c^2 + V)[I] + \frac{[\vec{\sigma} \cdot (\vec{\mathbf{p}} + e\vec{\mathbf{A}})]^2}{2m_0} \right\} \Psi = E\Psi \tag{53}$$

which reduces to

$$(E - m_0c^2)\Psi = \left\{ \frac{(\vec{\mathbf{p}} + e\vec{\mathbf{A}})^2}{2m_0}[I] + \mu_B \vec{\mathbf{B}} \cdot \vec{\sigma} + V[I] \right\} \Psi \tag{54}$$

$$\bar{E}\Psi = \{[H_0] + [H_B]\}\Psi \tag{55}$$

since it can be shown that

$$\begin{aligned} [\vec{\sigma} \cdot (\vec{\mathbf{p}} + e\vec{\mathbf{A}})]^2 &= (p_x + eA_x)^2 + (p_y + eA_y)^2 + (p_z + eA_z)^2 && (56) \\ &+ i\sigma_z \left(-ie\hbar \frac{\partial A_y}{\partial x} + ie\hbar \frac{\partial A_x}{\partial y} \right) && (57) \\ &+ i\sigma_y \left(-ie\hbar \frac{\partial A_x}{\partial z} + ie\hbar \frac{\partial A_z}{\partial x} \right) && (58) \\ &+ i\sigma_x \left(-ie\hbar \frac{\partial A_z}{\partial y} + ie\hbar \frac{\partial A_y}{\partial z} \right) && (59) \\ &= [\vec{\mathbf{p}} + e\vec{\mathbf{A}}]^2 + e\hbar(\boldsymbol{\nabla} \times \vec{\mathbf{A}}) \cdot \vec{\sigma} && (60) \\ &= (\vec{\mathbf{p}} + e\vec{\mathbf{A}})^2[I] + 2m_0\mu_B \vec{\mathbf{B}} \cdot \vec{\sigma} && (61) \end{aligned}$$

where we have used the fact that $\mu_B = e\hbar/2m_0$ and $\vec{\mathbf{B}} = \boldsymbol{\nabla} \times \vec{\mathbf{A}}$.

The second of the two equations in Eq.52 will yield the same result provided we make the transformation $m_0 \to -m_0$. This shows that the second equation applies to particles with negative mass, namely anti-matter. The energy separation (from the dispersion relation using Eq.29 and $p = \hbar k$) between the two is $2m_0c^2$ which is $\sim 1\,\text{MeV}$ for a free electron. These energy scales are seldom encountered in solid state physics, which is why anti-matter is usually of concern only in high energy physics.

2 On Bloch Sphere

The Bloch sphere concept is a useful tool to represent the actions of various quantum-mechanical operators on a spinor. It is particularly useful when describing the action of a spatially uniform external (including time-dependent) magnetic field on the spin [5] through the derivation of the Rabi formula. Bloch sphere concepts are also frequently invoked in discussions of spin-based quantum computing. A sound understanding of this notion is thus imperative to comprehend the literature in that field.

2.1 About "Qubit"

Quantum computers do not process classical binary bits 0 and 1, but instead process quantum bits which are coherent superpositions of both 0 and 1. A quantum computer derives its immense power from this superposition. It was realized quite some time back that the spin polarization of an electron is the ideal physical implementation of a qubit since spin polarization can survive in a coherent superposition of two orthogonal states for a relatively long time. These two orthogonal states (i.e., states with anti-parallel spin polarizations) will represent the classical bits 0 and 1.

Let us begin by writing the 2-component wavefunction representing an arbitrary spin state below:

$$\psi(\mathbf{X}) = \begin{bmatrix}\phi_1\\ \phi_2\end{bmatrix} \tag{62}$$

$$= \phi_1 \begin{bmatrix}1\\ 0\end{bmatrix} + \phi_2 \begin{bmatrix}0\\ 1\end{bmatrix} \tag{63}$$

$$= \phi_1 \left|+\right\rangle_z + \phi_2 \left|-\right\rangle_z \tag{64}$$

with

$$|\phi_1|^2 + |\phi_2|^2 = 1 \tag{65}$$

for $\psi(\mathbf{X})$ to be properly normalised.

The quantities ϕ_1 and ϕ_2 are complex quantities with both a magnitude and a phase. To maintain a coherent superposition state, we have to maintain the phase relationship between ϕ_1 and ϕ_2 until the qubit is "read" and collapses to either the $+z$ or the $-z$ state*. Spin couples relatively weakly to its surroundings, thus the coupling to the environment does not destroy the phase coherence of spin (phase relationship between ϕ_1 and ϕ_2) as rapidly as it does in the case of charge.

It is conventional to denote the $+z$-polarized state as representative of the classical bit 0, and the $-z$-polarized state as bit 1. Thus, the spinor ψ can be interpreted as a qubit since it has the exact mathematical form of a coherent superposition of bits 0 and 1, i.e.

$$\psi(\mathbf{X}) = \phi_1 \left|0\right\rangle + \phi_2 \left|1\right\rangle \tag{66}$$

Just as complex numbers have a nice powerful geometrical representation in the complex $\mathcal{C}$ plane, the spinors or qubits have an equilvalent representation in $\mathcal{C}^2$ in the form of the Bloch sphere.

2.2 Preliminary Concepts

2.2.1 The Spin Operator along an Arbitrary Direction

We have established in the previous chapter that an electron's spin is described by the operator:

$$\vec{\mathbf{S}} = \frac{\hbar}{2}\vec{\sigma} \tag{67}$$

A measurement of the spin component along an arbitrary direction characterized by a unit vector $\hat{\mathbf{n}}$ will then yield results given by the eigenvalues of the operator:

$$\vec{\mathbf{S}} \cdot \hat{\mathbf{n}} \tag{68}$$

and these eigenvalues are $\pm\frac{\hbar}{2}$, irrespective of the direction of the unit vector $\hat{\mathbf{n}}$.

This arises from Pauli's very definition for the $\vec{\mathbf{S}}$ operator in Chapter 1, although it can be proven by first recognising the following equality for the Pauli spin matrices [6]:

$$(\vec{\sigma}\cdot\vec{\mathbf{a}})(\vec{\sigma}\cdot\vec{\mathbf{b}}) = i\vec{\sigma}\cdot(\vec{\mathbf{a}}\times\vec{\mathbf{b}}) + \vec{\mathbf{a}}\cdot\vec{\mathbf{b}}\mathbf{I} \tag{69}$$

where $\mathbf{I}$ is the 2×2 identity matrix and $\vec{\mathbf{a}}$ and $\vec{\mathbf{b}}$ are arbitrary three dimensional vectors in real space $\mathcal{R}^3$.

If the vectors $\vec{\mathbf{a}}$ and $\vec{\mathbf{b}}$ are equal to a unit vector $\hat{\mathbf{n}}$, then the equality above reduces to

$$(\vec{\sigma}\cdot\hat{\mathbf{n}})^2 = \mathbf{I} \tag{70}$$

i.e., the square of any component of $\vec{\sigma}$ is equal to the unit 2×2 matrix. Hence, the eigenvalues of $\vec{\sigma}\cdot\hat{\mathbf{n}}$ are ± 1, and therefore (from Eq.67) the eigenvalues of the operator $\vec{\mathbf{S}}\cdot\hat{\mathbf{n}}$ must be $\pm\frac{\hbar}{2}$. In other words, the measurement of the spin angular momentum along any arbitrary axis always yields the values $\pm\frac{\hbar}{2}$.

2.2.2 Eigenvectors of $\vec{\sigma}\cdot\hat{\mathbf{n}}$

Let us derive the explicit analytical expressions for the eigenvectors of $\vec{\sigma}\cdot\hat{\mathbf{n}}$ corresponding to the eigenvalues $+1$ and -1.

We first consider the following operators

$$\frac{1}{2}(1\pm\vec{\sigma}\cdot\hat{\mathbf{n}}) \tag{71}$$

acting on an arbitrary spinor $|\chi\rangle$. If we operate on that with the an additional operator $\vec{\sigma}\cdot\hat{\mathbf{n}}$, we get

$$(\vec{\sigma}\cdot\hat{\mathbf{n}})\left[\frac{1}{2}(1\pm\vec{\sigma}\cdot\hat{\mathbf{n}})\,|\chi\rangle\right] = \frac{1}{2}(\vec{\sigma}\cdot\hat{\mathbf{n}})\,|\chi\rangle \pm \frac{1}{2}(\vec{\sigma}\cdot\hat{\mathbf{n}})^2\,|\chi\rangle \tag{72}$$

$$= \pm\left[\frac{1}{2}(1\pm\vec{\sigma}\cdot\hat{\mathbf{n}})\,|\chi\rangle\right] \tag{73}$$

Thus, we have shown that for any $|\chi\rangle$, $\frac{1}{2}(1\pm\vec{\sigma}\cdot\hat{\mathbf{n}})\,|\chi\rangle$ are eigenvectors of $\vec{\sigma}\cdot\hat{\mathbf{n}}$ with eigenvalues ± 1.

Then, we make use of the identity

$$\frac{1}{2}(1\pm\vec{\sigma}\cdot\hat{\mathbf{n}}) = \frac{1}{2}\left[1\pm\sigma_z n_z \pm \frac{1}{2}(\sigma_x + i\sigma_y)(n_x - in_y) \pm \frac{1}{2}(\sigma_x - i\sigma_y)(n_x + in_y)\right] \tag{74}$$

Writing $\hat{\mathbf{n}}$ in spherical coordinates with polar angle θ and azimuthal angle ϕ, i.e.

$$(n_x, n_y, n_z) = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta) \tag{75}$$

we yield

$$n_x \pm in_y = \sin\theta e^{\pm i\phi} \tag{76}$$

which lets us rewrite the identity in Eq.74 as

$$\frac{1}{2}(1\pm\vec{\sigma}\cdot\hat{\mathbf{n}}) = \frac{1}{2}\left[1\pm\cos\theta\sigma_z \pm \frac{1}{2}(\sin\theta e^{-i\phi}\sigma_+ \pm \sin\theta e^{i\phi}\sigma_-)\right] \tag{77}$$

where we have denoted $\sigma_+ = \sigma_x + i\sigma_y$ and $\sigma_- = \sigma_x - i\sigma_y$.

Acting these operators on the spinor $|0\rangle$ will get us

$$\frac{1}{2}(1+\vec{\sigma}\cdot\hat{\mathbf{n}})\,|0\rangle = \cos\frac{\theta}{2}\left[\cos\frac{\theta}{2}\,|0\rangle + \sin\frac{\theta}{2}e^{i\phi}\,|1\rangle\right] \tag{78}$$

$$\frac{1}{2}(1-\vec{\sigma}\cdot\hat{\mathbf{n}})\,|0\rangle = \sin\frac{\theta}{2}\left[\sin\frac{\theta}{2}\,|0\rangle - \cos\frac{\theta}{2}e^{i\phi}\,|1\rangle\right] \tag{79}$$

where we have used simple half- and double-angle trigonometric identities in arriving at the last two lines.

It is easy to see then that the two spinors can be normalized by dividing the first by $\cos\frac{\theta}{2}$ and the second by $\sin\frac{\theta}{2}$. Thus, we introduce the normalised spinors

$$\left|\xi_n^+\right\rangle = \cos\frac{\theta}{2}\left|0\right\rangle + \sin\frac{\theta}{2}e^{i\phi}\left|1\right\rangle \tag{80}$$

$$\left|\xi_n^-\right\rangle = \sin\frac{\theta}{2}\left|0\right\rangle - \cos\frac{\theta}{2}e^{i\phi}\left|1\right\rangle \tag{81}$$

as eigenvectors of the operator $\vec{\sigma}\cdot\hat{\mathbf{n}}$ with eigenvalues $+1$ and -1, respectively.

We note the that spinor $|\xi_n^-\rangle$ can actually be obtained from the spinor $|\xi_n^+\rangle$ by making the following transformation:

$$\left|\xi_n^-\right\rangle = \left|\xi_n^+(\theta\to\pi-\theta,\phi\to\phi+\pi)\right\rangle \tag{82}$$

Hereafter, we adopt the common convention to use $|\xi_n^+\rangle$ to represent the most general form of the spinor by including an additional overall phase factor $e^{i\gamma}$ which will not affect any measurement made on the spinor:

$$\left|\xi_n^+\right\rangle = e^{i\gamma}\left[\cos\frac{\theta}{2}\left|0\right\rangle + \sin\frac{\theta}{2}e^{i\phi}\left|1\right\rangle\right] \tag{83}$$

Since $|\xi_n^+\rangle$ can be obtained by acting with the operator $\frac{1}{2}(1+\vec{\sigma}\cdot\hat{\mathbf{n}})$ on an arbitrary qubit $|\chi\rangle$, this operator is referred to as the projection operator in the direction $\hat{\mathbf{n}}$. Similarly, the operator $\frac{1}{2}(1-\vec{\sigma}\cdot\hat{\mathbf{n}})$ is the projection operator in the direction $-\hat{\mathbf{n}}$.

The relationship between the unit vector $\hat{\mathbf{n}}$ and the spinor $|\xi_n^+\rangle$ is represented geometrically using a sphere of radius 1 – the socalled Bloch sphere – where $\hat{\mathbf{n}}$ is the radius vector of the Bloch sphere. The surface of the sphere represents the vector space of the spinor $|\xi_n^+\rangle$, namely the eigenvector of $\vec{\sigma}\cdot\hat{\mathbf{n}}$ with eigenvalue $+1$. This pictorial representation is very useful when analyzing the action of 2×2 unitary matrices acting on the spinor $|\xi_n^+\rangle$ as actual rotations of the unit vector $\hat{\mathbf{n}}$ on the Bloch sphere.

2.3 Orthonormality in Diametrical Opposites

For an electron characterized by the spinor $|\xi_n^+\rangle$, it can be easily shown that the expectation values of the Pauli spin matrices are given by

$$\left\langle\xi_n^+\middle|\sigma_x\middle|\xi_n^+\right\rangle = \sin\theta\cos\phi \tag{84}$$

$$\left\langle\xi_n^+\middle|\sigma_y\middle|\xi_n^+\right\rangle = \sin\theta\sin\phi \tag{85}$$

$$\left\langle\xi_n^+\middle|\sigma_z\middle|\xi_n^+\right\rangle = \cos\theta \tag{86}$$

which are exactly the cartesian components of the unit vector $\hat{\mathbf{n}}$.

Similarly for $|\xi_n^-\rangle$, we obtain

$$\left\langle\xi_n^-\middle|\sigma_x\middle|\xi_n^-\right\rangle = -\sin\theta\cos\phi \tag{87}$$

$$\left\langle\xi_n^-\middle|\sigma_y\middle|\xi_n^-\right\rangle = -\sin\theta\sin\phi \tag{88}$$

$$\left\langle\xi_n^-\middle|\sigma_z\middle|\xi_n^-\right\rangle = -\cos\theta \tag{89}$$

which are the cartesian coordinates of a unit vector diametrically opposite to the previous unit vector $\hat{\mathbf{n}}$. Therefore, any two diametrically opposite points on the surface of the Bloch sphere can be thought of as representations for orthogonal eigenstates of the operator $\vec{\sigma}\cdot\hat{\mathbf{n}}$ with eigenvalues ± 1.

2.4 Relationship with Qubit

We can express the qubit $|\chi\rangle$ as a normalised column vector in $\mathcal{C}^2$:

$$|\chi\rangle = \begin{bmatrix}\alpha\\ \beta\end{bmatrix} \tag{90}$$

$$= \begin{bmatrix}|\alpha|e^{i\phi_\alpha}\\ |\beta|e^{i\phi_\beta}\end{bmatrix} \tag{91}$$

$$= e^{i\phi_\alpha}\begin{bmatrix}|\alpha|\\ |\beta|e^{i(\phi_\beta-\phi_\alpha)}\end{bmatrix} \tag{92}$$

which has the general form of $|\xi_n^+\rangle$ in Eq.83 for the following choice of parameters:

$$\gamma = \phi_\alpha \tag{93}$$

$$\theta = 2\arctan\left(\frac{\sqrt{1-|\alpha|^2}}{|\alpha|}\right) \tag{94}$$

$$\phi = \phi_\beta - \phi_\alpha \tag{95}$$

2.5 Geometric Properties

2.5.1 North-South Spinors

From Eq.83, it is obvious that the state $|0\rangle$ can be written as

$$|0\rangle = \left|\xi_n^+(\theta = 0, \phi, \gamma)\right\rangle \tag{96}$$

and the state $|1\rangle$ as

$$|1\rangle = \left|\xi_n^+(\theta = \pi, \phi, \gamma)\right\rangle \tag{97}$$

The fact that ϕ and γ are arbitrary is irrelevant since observables should not depend on the overall phase of the spinor. This interpretation is consistent with associating the spinor $|0\rangle$ with the point representing the north pole on the Bloch sphere and $|1\rangle$ with the south pole on the Bloch sphere – in agreement with our previous findings that orthogonal states are diametrically opposite on the Bloch sphere.

2.5.2 At the "45th Parallel"

The Hadamard matrix is one of the most widely used matrix in the design of quantum logic gates and is given by

$$H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \tag{98}$$

It is easy to check that one of the two eigenvectors of the Hadamard matrix is given by

$$|\chi\rangle_H = \cos\left(\frac{\pi}{8}\right)|0\rangle + \sin\left(\frac{\pi}{8}\right)|1\rangle \tag{99}$$

Using our expression for qubit in Eq.92, we find that

$$\theta = \frac{\pi}{4} \tag{100}$$

$$\phi = 0 \tag{101}$$

$$\gamma = 2\pi n, \;\; n = \mathcal{Z} \tag{102}$$

Hence the eigenvector of the Hadamard matrix is in the x-z plane, halfway between the north pole and the positive x-axis. It is then easy to show that the other eigenvector of the Hadamard matrix is located diametrically opposite to this unit vector.

2.6 Spin Flip Matrix

Let us consider a 2×2 matrix $\mathbf{M}$ which changes $|\xi_n^-\rangle$ into $|\xi_n^+\rangle$:

$$\left|\xi_n^+\right\rangle = \mathbf{M}\left|\xi_n^-\right\rangle \tag{103}$$

$$e^{i\gamma}\begin{bmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2}e^{i\phi} \end{bmatrix} = \mathbf{M}e^{i\gamma}\begin{bmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2}e^{i\phi} \end{bmatrix} \tag{104}$$

Evidently, we find

$$\mathbf{M} = \begin{bmatrix} 0 & -e^{-i\phi} \\ e^{i\phi} & 0 \end{bmatrix} \tag{105}$$

The spin flip matrix $\mathbf{M}$ can be written as a product of some well-known 2×2 matrices:

$$\mathbf{M} = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix} \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & e^{-i\phi} \end{bmatrix} \tag{106}$$

or more compactly,

$$\mathbf{M} = e^{-i\frac{\pi}{2}} P(\phi) \sigma_y P(-\phi) \tag{107}$$

where $P(\phi) = \begin{bmatrix} 1 & 0 \\ 0 & e^{i\phi} \end{bmatrix}$ is the phase shift matrix.

2.7 Pauli Matrices Revisited

For any unitary matrix $\mathbf{A}$, we have the following identity:

$$e^{i\theta\mathbf{A}} = \cos\theta \mathbf{I} + i \sin\theta \mathbf{A} \tag{108}$$

which is the generalisation to operators of the Euler relation for complex numbers $e^{iz} = \cos z + i \sin z$.

It is easy to prove the above. We first start with the Taylor series expansion

$$\begin{aligned} e^{i\theta\mathbf{A}} &= \mathbf{I} + (i\theta)\mathbf{A} + \frac{(i\theta)^2\mathbf{A}^2}{2!} + \frac{(i\theta)^3\mathbf{A}^3}{3!} + \frac{(i\theta)^4\mathbf{A}^4}{4!} + \cdots && (109) \\ &= \left[1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} - \cdots + (-1)^k \frac{\theta^{2k}}{(2k)!}\right]\mathbf{I} && (110) \\ &\quad + i\left[\theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \cdots + (-1)^k \frac{i\theta^{2k+1}}{(2k+1)!}\right]\mathbf{A} && (111) \end{aligned}$$

which gives precisely Eq.108 when we make the substitutions:

$$\sin x = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k+1}}{(2k+1)!} \tag{112}$$

$$\cos x = \sum_{k=0}^{\infty} (-1)^k \frac{x^{2k}}{(2k)!} \tag{113}$$

Now, let us state without proof [3] that the matrices characterising the rotations of a general spinor around the individual axes are

$$R_x(\theta) = \begin{bmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \tag{114}$$

$$R_y(\theta) = \begin{bmatrix} \cos\frac{\theta}{2} & -\sin\frac{\theta}{2} \\ \sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{bmatrix} \tag{115}$$

$$R_z(\theta) = \begin{bmatrix} e^{-i\frac{\theta}{2}} & 0 \\ 0 & e^{i\frac{\theta}{2}} \end{bmatrix} \tag{116}$$

Using the identity in Eq.108, these rotation operators can be rewritten as

$$R_x(\theta) = e^{-i\frac{\theta}{2}\sigma_x} \tag{117}$$

$$R_y(\theta) = e^{-i\frac{\theta}{2}\sigma_y} \tag{118}$$

$$R_z(\theta) = e^{-i\frac{\theta}{2}\sigma_z} \tag{119}$$

Because the Pauli matrices constitute the building blocks to describe rotations on the Bloch sphere with the x, y or z-axis as the axis of rotations, they are referred to as the generators of the rotations in the Hilbert space of spinors associated with spin-1/2 particles [2].

3 Adventures in Bloch Sphere

In this chapter, we consider the general approach used to calculate the time evolution of the probability of a spinor reaching a particular location on the Bloch sphere from another location, when subjected to the simultaneous actions of two spatially uniform magnetic fields. One of these fields is static (time-independent) and directed along a specific axis, while the other is time-dependent, has a different amplitude, and rotates in the plane perpendicular to the first magnetic field.

3.1 Spin-1/2 Particles and the Larmor Precession

Let us recall the Ehrenfest theorem for an operator $\mathbf{A}$ in quantum mechanics [7]:

$$\frac{\mathrm{d}\langle\mathbf{A}\rangle}{\mathrm{d}t} = \frac{1}{i\hbar}\langle[\mathbf{HA}]\rangle + \left\langle\frac{\partial\mathbf{A}}{\partial t}\right\rangle \tag{120}$$

where $\mathbf{H}$ is the usual Hamiltonian, and square bracket denotes the familiar commutator relation.

We can use the Ehrenfest theorem to calculate the time evolution of the spin of an electron in a spatially uniform but time-dependent magnetic field $\vec{\mathbf{B}}(t)$. In this case, we have for the Hamiltonian (see Chap.1.2.1):

$$\mathbf{H} = H_0 - \frac{g}{2}\mu_B\vec{\mathbf{B}}\cdot\vec{\sigma} \tag{121}$$

We have demonstrated in previous chapter that the spin of an electron can be characterised by the Pauli spin matrices. Thus,

$$i\hbar\frac{\mathrm{d}\langle\sigma_x\rangle}{\mathrm{d}t} = -\frac{g\mu_B}{2}[B_y\langle(\sigma_y\sigma_x-\sigma_x\sigma_y)\rangle + B_z\langle(\sigma_z\sigma_x-\sigma_x\sigma_z)\rangle] \tag{122}$$

where we have ignored the last term since σ_x is time-independent.

Recall the well-known properties of the Pauli spin matrices:

$$\sigma_x\sigma_y = -\sigma_y\sigma_x = i\sigma_z \tag{123}$$
$$\sigma_z\sigma_x = -\sigma_x\sigma_z = i\sigma_y \tag{124}$$

Hence, we can rewrite Eq.122 as

$$\frac{\mathrm{d}\langle\sigma_x\rangle}{\mathrm{d}t} = \frac{g\mu_B}{\hbar}(B_y\langle\sigma_z\rangle - B_z\langle\sigma_y\rangle) \tag{125}$$

Likewise, we can obtain equivalent relations for $\frac{\mathrm{d}\langle\sigma_y\rangle}{\mathrm{d}t}$ and $\frac{\mathrm{d}\langle\sigma_z\rangle}{\mathrm{d}t}$:

$$\frac{\mathrm{d}\langle\sigma_y\rangle}{\mathrm{d}t} = \frac{g\mu_B}{\hbar}(B_z\langle\sigma_x\rangle - B_x\langle\sigma_z\rangle) \tag{126}$$
$$\frac{\mathrm{d}\langle\sigma_z\rangle}{\mathrm{d}t} = \frac{g\mu_B}{\hbar}(B_x\langle\sigma_y\rangle - B_y\langle\sigma_x\rangle) \tag{127}$$

This set of coupled equations can be written in a matrix form as

$$\frac{\mathrm{d}}{\mathrm{d}t}\begin{bmatrix}\langle\sigma_x\rangle\\\langle\sigma_y\rangle\\\langle\sigma_z\rangle\end{bmatrix} = \frac{g\mu_B}{\hbar}\begin{bmatrix}0 & -B_z & B_y\\ B_z & 0 & -B_x\\ -B_y & B_x & 0\end{bmatrix}\begin{bmatrix}\langle\sigma_x\rangle\\\langle\sigma_y\rangle\\\langle\sigma_z\rangle\end{bmatrix} \tag{128}$$

or more compactly in vectorial form:

$$\frac{\mathrm{d}\langle\vec{\sigma}\rangle}{\mathrm{d}t} = \frac{g\mu_B}{\hbar}(\vec{\mathbf{B}}\times\langle\vec{\sigma}\rangle) \tag{129}$$
$$= \vec{\mathbf{\Omega}}\times\langle\vec{\sigma}\rangle \tag{130}$$

where $\vec{\mathbf{\Omega}} = \frac{g\mu_B}{\hbar}\vec{\mathbf{B}}$, and in the case of a free electron $= \frac{e\vec{\mathbf{B}}}{m_0}$ (because $g_{\text{free}} = 2, \mu_B = \frac{e\hbar}{2m_0}$).

$\vec{\mathbf{\Omega}}$ is the well known Larmor precession frequency. If the magnetic field is time-independent, then the Larmor precession frequency is also time-independent; otherwise, it follows the time dependence of the magnetic field.

In upholding the rigor and precision of our present discussion, we should use $S_n = (\hbar/2)\sigma_n$ as the operator for a component of the spin angular momentum along some coordinate axis. Nevertheless, it is easy to see that Eq.130 is simply

$$\frac{\mathrm{d}\left\langle \vec{\mathbf{S}} \right\rangle}{\mathrm{d}t} = \frac{g\mu_B}{\hbar}(\vec{\mathbf{B}} \times \left\langle \vec{\mathbf{S}} \right\rangle) \tag{131}$$

$$= \vec{\boldsymbol{\Omega}} \times \left\langle \vec{\mathbf{S}} \right\rangle \tag{132}$$

otherwise known as the Larmor equation describing Larmor precession of a spin about a magnetic field.

3.2 The Rabi Formula

In most textbooks, the Rabi formula is derived by solving the time-dependent Pauli equation (Eq.19) with a clever selection of the reference frame to describe the time-evolution of the 2-component spinor wavefunction. Here, we shall use a different approach based on the concept of the Bloch sphere instead.

3.2.1 A Complicated Rotation - 2 B-fields

In the previous section, we derived the equation of motion of a spinor in an arbitrary spatially uniform magnetic field $\vec{\mathbf{B}}_0$, and showed that the spinor will precess about the field in a cone with an angular frequency that is proportional to the strength of the magnetic field. Getting this spinor to flip diametrically will involve a second rotating magnetic field $\vec{\mathbf{B}}_1$ (Chap. 4 of [3]). We can of course choose to only have a single magnetic field acting orthogonally to the spinor to achieve the same results but let us instead choose to over-complicate matter for now.

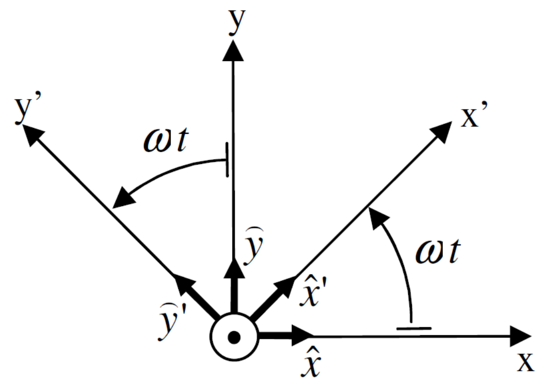

Figure 1: Illustration of the two reference frames used to described the temporal evolution of a spinor.

Consider a fixed reference frame with Cartesian coordinates (x, y, z) and a second time-varying reference frame $(x'(t), y'(t), z'(t))$ obtained from the initial reference frame through an anti-clockwise rotation around the z-axis at an angular frequency ω. We chose this second reference frame to coincide with our rotating magnetic field $\vec{\mathbf{B}}_1$. It is easy to see then that the relationship between the unit vector in the unprimed and primed reference frames is given by:

$$\hat{\mathbf{x}}' = \cos\omega t\hat{\mathbf{x}} + \sin\omega t\hat{\mathbf{y}} \tag{133}$$

$$\hat{\mathbf{y}}' = -\sin\omega t\hat{\mathbf{x}} + \cos\omega t\hat{\mathbf{y}} \tag{134}$$

$$\hat{\mathbf{z}}' = \hat{\mathbf{z}} \tag{135}$$

Using these relations, any three-dimensional vector $\hat{\mathbf{n}}$ when decomposed in the two reference frames are related as follows:

$$\hat{\mathbf{n}}' = \begin{bmatrix} n'_x \\ n'_y \\ n'_z \end{bmatrix} = [A] \begin{bmatrix} n_x \\ n_y \\ n_z \end{bmatrix} = [A]\hat{\mathbf{n}} \tag{136}$$

where (n_x, n_y, n_z) and (n'_x, n'_y, n'_z) are the components in the unprimed and primed reference frames respectively, and $[A]$ is given by

$$[A] = \begin{bmatrix} \cos\omega t & \sin\omega t & 0 \\ -\sin\omega t & \cos\omega t & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{137}$$

Earlier, we saw that when a spinor is subjected to a spatially uniform time dependent magnetic field, its time evolution is given by Eq.128. Therefore, in the unprimed reference frame, we have

$$\frac{\mathrm{d}\hat{\mathbf{n}}}{\mathrm{d}t} = [X]\hat{\mathbf{n}} \tag{138}$$

where the matrix $[X]$ is given explicitly by the 3×3 matrix in Eq.128.

Naturally, we then ask what is the analytical form of the matrix $[X']$ such that

$$\frac{\mathrm{d}\hat{\mathbf{n}}'}{\mathrm{d}t} = [X']\hat{\mathbf{n}}' \tag{139}$$

which describes the time evolution of the spinor in our rotating frame. From Eq,136, we get

$$\frac{\mathrm{d}\hat{\mathbf{n}}}{\mathrm{d}t} = [A]^{-1}\frac{\mathrm{d}\hat{\mathbf{n}}'}{\mathrm{d}t} + \frac{\mathrm{d}[A]^{-1}}{\mathrm{d}t}\hat{\mathbf{n}}' \tag{140}$$

where we can easily find $[A]^{-1}$ to be

$$[A]^{-1} = \begin{bmatrix} \cos\omega t & -\sin\omega t & 0 \\ \sin\omega t & \cos\omega t & 0 \\ 0 & 0 & 1 \end{bmatrix} \tag{141}$$

Therefore,

$$[A]^{-1}\frac{\mathrm{d}\hat{\mathbf{n}}'}{\mathrm{d}t} + \frac{\mathrm{d}[A]^{-1}}{\mathrm{d}t}\hat{\mathbf{n}}' = [X]\hat{\mathbf{n}} \tag{142}$$

$$= [X][A]^{-1}\hat{\mathbf{n}}' \tag{143}$$

which can in turn be rearranged as follows

$$\frac{\mathrm{d}\hat{\mathbf{n}}'}{\mathrm{d}t} = \left\{[A][X][A]^{-1} - [A]\frac{\mathrm{d}[A]^{-1}}{\mathrm{d}t}\right\}\hat{\mathbf{n}}' \tag{144}$$

Comparing the last equation with Eq.139, we have found

$$[X'] = [A][X][A]^{-1} - [A]\frac{\mathrm{d}[A]^{-1}}{\mathrm{d}t} \tag{145}$$

Suppose our spinor is subjected to the following magnetic fields $\vec{\mathbf{B}}_0$ and $\vec{\mathbf{B}}_1$:

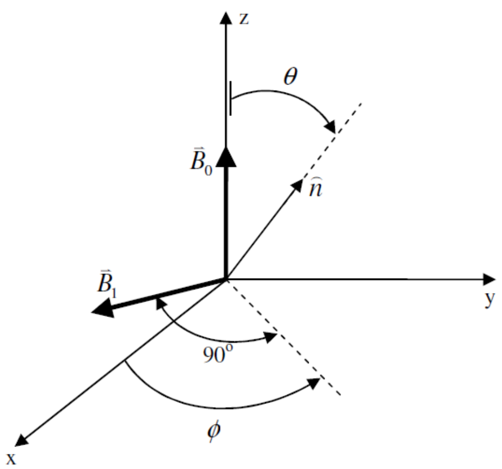

Figure 2: Magnetic fields acting on the spinor.

The resultant $\vec{\mathbf{B}}$ field can be written as

$$\vec{\mathbf{B}} = (B_1 \cos\omega t, B_1 \sin\omega t, B_0) \tag{146}$$

Thus, using our expressions for $[X]$, $[A]$, and $[A]^{-1}$, it is trivial to show that the matrix $[X']$ can be written as

$$[X'] = \begin{bmatrix} 0 & \omega-\omega_0 & 0 \\ -(\omega-\omega_0) & 0 & -\omega_1 \\ 0 & \omega_1 & 0 \end{bmatrix} \tag{147}$$

where

$$\omega_0 = \frac{g\mu_B B_0}{\hbar} \tag{148}$$

$$\omega_1 = \frac{g\mu_B B_1}{\hbar} \tag{149}$$

Note that ω_0 is the Larmor frequency associated with the static magnetic field in the z-axis and ω_1 is the Larmor frequency associated with the time varying magnetic field rotating in the x-y plane.

3.2.2 Time Evolution of Spinor

Since the elements of the matrix $[X']$ are independent of time, the solution to Eq.139 is then given by

$$\hat{\mathbf{n}}'(t) = e^{[Q(t)]}\hat{\mathbf{n}}'(0) \tag{150}$$

where

$$[Q(t)] = \int_0^t dt'\,[X'] \tag{151}$$

$$= \begin{bmatrix} 0 & (\omega-\omega_0)t & 0 \\ -(\omega-\omega_0)t & 0 & -\omega_1 t \\ 0 & \omega_1 t & 0 \end{bmatrix} \tag{152}$$

Now, suppose we have the matrix $[S(t)]$ which diagonalizes $[Q(t)]$, i.e.,

$$[\Lambda(t)] = [S(t)]^{-1}[Q(t)][S(t)] = \mathrm{diag}(\lambda_1(t), \lambda_2(t), \lambda_3(t)) \tag{153}$$

where $\lambda_i (i = 1, 2, 3)$ are the three eigenvalues of the matrix $[Q(t)]$.

Hence, we have

$$e^{[Q(t)]} = e^{[S(t)][\Lambda(t)][S(t)]^{-1}} \tag{154}$$

$$= [I] + [S][\Lambda][S]^{-1} + \frac{1}{2!}\left([S][\Lambda][S]^{-1}\right)^2 + \ldots \tag{155}$$

$$= [I] + [S]\left([\Lambda] + \frac{[\Lambda]^2}{2!} + \frac{[\Lambda]^3}{3!} + \ldots\right)[S]^{-1} \tag{156}$$

$$= [S]e^{[\Lambda(t)]}[S]^{-1} \tag{157}$$

Therefore, this leads to

$$\hat{\mathbf{n}}(t) = [U]\hat{\mathbf{n}}(0) \tag{158}$$

$$= \left\{[A(t)]^{-1}\left[[S(t)]e^{[\Lambda(t)]}[S(t)]^{-1}\right]A(0)\right\}\hat{\mathbf{n}}(0) \tag{159}$$

This last equation describes the time evolution of the spinor on the Bloch sphere in the initial fixed frame of reference.

We continue on our mathematical journey, calculating explicitly the matrix $[S]$ next. Hereafter, we use the shorthand notations $\alpha = (\omega - \omega_0)t$ and $\beta = -\omega_1 t$. The eigenvalues λ_i of the matrix $[Q(t)]$ are easily determined to be

$$\lambda_1 = 0 \tag{160}$$

$$\lambda_2 = i\sqrt{\alpha^2+\beta^2} \tag{161}$$

$$\lambda_3 = -i\sqrt{\alpha^2+\beta^2} \tag{162}$$

and the respective eigenvectors are

$$\vec{\mathbf{q}}_1 = \left[\frac{\beta}{\alpha}, 0, 1\right] \tag{163}$$

$$\vec{\mathbf{q}}_2 = \left[-\frac{\alpha}{\beta}, \frac{-i\sqrt{\alpha^2+\beta^2}}{\beta}, 1\right] \tag{164}$$

$$\vec{\mathbf{q}}_3 = \left[-\frac{\alpha}{\beta}, \frac{i\sqrt{\alpha^2+\beta^2}}{\beta}, 1\right] \tag{165}$$

Matrix $[S]$ must then have column vectors equal to the three eigenvectors of the matrix $[Q]$ in order to diagonalise it (Eq.153):

$$[S] = \begin{bmatrix} \beta/\alpha & -\alpha/\beta & -\alpha/\beta \\ 0 & -i\sqrt{\alpha^2+\beta^2}/\beta & i\sqrt{\alpha^2+\beta^2}/\beta \\ 1 & 1 & 1 \end{bmatrix} \tag{166}$$

It is trivial to show that its inverse is

$$[S]^{-1} = \begin{bmatrix} \alpha\beta/\left[\alpha^2+\beta^2\right] & 0 & \alpha^2/\left[\alpha^2+\beta^2\right] \\ -0.5\alpha\beta/\left[\alpha^2+\beta^2\right] & 0.5i\beta/[\sqrt{\alpha^2+\beta^2}] & 0.5\beta^2/\left[\alpha^2+\beta^2\right] \\ -0.5\alpha\beta/\left[\alpha^2+\beta^2\right] & -0.5i\beta/[\sqrt{\alpha^2+\beta^2}] & 0.5\beta^2/\left[\alpha^2+\beta^2\right] \end{bmatrix} \tag{167}$$

Alas, we can now write for the matrix $[U]$:

$$[U] = \begin{bmatrix} g(\delta,\chi)\sin\omega t + h(\delta,\chi)\cos\omega t & g(\delta,\chi)\cos\omega t - \cos\delta\sin\omega t & [f(\delta)\cos\omega t\cos\chi - \sin\delta\sin\omega t]\sin\chi \\ -g(\delta,\chi)\cos\omega t + h(\delta,\chi)\sin\omega t & g(\delta,\chi)\sin\omega t + \cos\delta\cos\omega t & [f(\delta)\sin\omega t\cos\chi + \sin\delta\cos\omega t]\sin\chi \\ f(\delta)\cos\chi\sin\chi & -\sin\delta\sin\chi & \cos^2\chi + \sin^2\chi\cos\delta \end{bmatrix} \tag{168}$$

where we have denoted

$$\begin{aligned} \delta &= \sqrt{\alpha^2+\beta^2} \\ &= \sqrt{(\omega-\omega_0)^2 + \omega_1^2}\, t \\ f(\delta) &= 1 - \cos\delta \\ h(\delta,\chi) &= \cos\delta\cos^2\chi + \sin^2\chi \\ g(\delta,\chi) &= \sin\delta\cos\chi \\ \chi &= \operatorname{atan}\left[\omega_1/\left(\omega_0-\omega\right)\right] \\ \sin^2\chi &= \frac{\omega_1^2}{\omega_1^2 + \left[\omega_0-\omega\right]^2} \end{aligned} \tag{169}$$

3.2.3 Finding Probability - The Rabi Formula

The probability for any arbitrary spinor (see Eq.83) to be eventually located at the south pole is given by:

$$|\left\langle 1|\xi_n^+\right\rangle|^2 = \sin^2\left(\frac{\theta(t)}{2}\right) \tag{170}$$

$$= \frac{1-\cos\theta(t)}{2} \tag{171}$$

$$= \frac{1-n_z(t)}{2} \tag{172}$$

For ease of calculation, let us start with our spinor located at the north pole on the Bloch sphere at $t=0$. Hence, $\hat{\mathbf{n}}(0) = ((n_x(0), n_y(0), n_z(0)) = (0,0,1)$. We can find $n_z(t)$ from Eq.159 and substitute that in the above equation to yield

$$\sin^2\left(\frac{\theta(t)}{2}\right) = \frac{\sin^2\chi(t)}{2}[1-\cos\delta(t)] \tag{173}$$

This is known as the Rabi formula and it indicates that the probability of spin flip reaches a maximum of $\sin^2\chi$ and only achieves unity when the following resonance condition is satisfied

$$\sin^2\chi(t) = 1 \tag{174}$$

$$\omega = \omega_0 \tag{175}$$

The physical meaning translates to the magnetic field B_1 in the $(x-y)$ plane rotating at a frequency ω equal to the Larmor frequency $\frac{g\mu_B B_0}{\hbar}$ in order for the spinor to reach the south pole.

3.3 Spin Flip Time

The magnetic field $\vec{\mathbf{B}}_1$ must rotate in the (x-y) plane with an angular frequency ω_0, which is the Larmor frequency associated with the static field $\vec{\mathbf{B}}_0$, in order to guarantee a spin flip. The spinor $\hat{\mathbf{n}}$ will periodically visit the north and south poles of the Bloch sphere with a frequency equal to the Larmor frequency of the field in the (x-y) plane, which is ω_1. Therefore, the time that elapses between two consecutive visits of either pole is $T = 2\pi/\omega_1$ and the time required to switch from one pole to the other, which is the time required for the spin to flip, is

$$t_s = \frac{T}{2} \tag{176}$$

$$= \frac{\pi}{\omega_1} \tag{177}$$

$$= \frac{\pi\hbar}{g\mu_B B_1} \tag{178}$$

This time is inversely proportional to the strength of the field B_1. The derivation of Rabi's formula was based on the general Eq.159 which allows a direct calculation of the time dependence of the probability of a spin transfer between any two points of the Bloch sphere, starting at a location at time $t = 0$ other than the north pole, which is usually the case derived in most textbooks based on a direct solution of the time-dependent Schrödinger equation.

4 On Purity in Quantum Mechanics

4.1 The Density Matrix

4.1.1 Pure vs. Mixed States

4.2 Time Evolution of Density Matrix

4.3 Relaxation Times & Bloch Equations

5 Spin Orbit Coupling (SOC)

5.1 Rashba Interfacial Interaction

5.2 Dresselhaus Bulk Interaction

6 Excursions with SOC

References

[1] Richard Fitzpatrick. Orbital angular momentum, jan 2016. URL https://farside.ph.utexas.edu/teaching/qm/Quantum/node39.html.

[2] R.P. Feynman; R.B. Leighton; M. Sands. *The Feynman Lectures on Physics*, volume 2. Addison-Wesley, 1964. Chapter 34.

[3] Supriyo Bandyopadhyay; Marc Cahay. *Introduction to Spintronics.* CRC Press, second edition, 2008.

[4] R. E. Moss. *Advanced Molecular Quantum Mechanics, An Introduction to Relativistic Quantum Mechanics and the Quantum Theory of Radiation.* Chapman and Hall Ltd, first edition, 1973. Chapter 8, Page 119.

[5] Shi-Liang Zhu; Z. D. Wang; Yong-Dong Zhang. Nonadiabatic noncyclic geometric phase of a spin-1/2 particle subject to an arbitrary magnetic field. *Physical Review B*, 61(2), jan 2000.

[6] Pauli matrices. URL https://en.wikipedia.org/wiki/Pauli_matrices.

[7] Ehrenfest theorem. URL https://en.wikipedia.org/wiki/Ehrenfest_theorem.