3

Manipulating qubits

In the preceding chapter we studied a qubit at a particular instant of time and we neglected, for example, the qubit evolution between preparation and measurement. As we have seen, in a Hilbert space $\mathcal{H}$ with an orthonormal basis formed of two vectors $|0\rangle$ and $|1\rangle$, this qubit is described by a normalized vector $|\varphi\rangle$:

$$|\varphi\rangle = \lambda|0\rangle + \mu|1\rangle, \qquad |\lambda|^2 + |\mu|^2 = 1. \tag{3.1}$$

In this chapter, we want to examine the time evolution of this qubit, in order to understand how it can be manipulated. We shall see that Rabi oscillations (Section 3.3) provide the basic mechanism that allows us to manipulate qubits.

3.1 The Bloch sphere, spin 1/2

Before turning to time evolution, let us give a somewhat more general description of a qubit and of its physical realizations. In writing down (3.1) we have used an orthonormal basis $\{|0\rangle, |1\rangle\}$ of $\mathcal{H}$, and the coefficients λ and μ can be parametrized, taking into account the arbitrariness of the phase, as

$$\lambda = \mathrm{e}^{-\mathrm{i}\phi/2} \cos\frac{\theta}{2}, \qquad \mu = \mathrm{e}^{\mathrm{i}\phi/2} \sin\frac{\theta}{2}. \tag{3.2}$$

The two angles θ and ϕ can be taken as the polar and azimuthal angles which parametrize the location of a point on the surface of a sphere of unit radius called the *Bloch sphere* (or the Poincaré sphere for the photon); see Fig. 3.1.

Returning to the photon polarization and identifying $|0\rangle \to |x\rangle$ and $|1\rangle \to |y\rangle$, the states $|x\rangle$ and $|y\rangle$ correspond to the north and south poles of the sphere:

$$|x\rangle : \ \theta = 0, \ \phi \text{ undetermined}, \qquad |y\rangle : \ \theta = \pi, \ \phi \text{ undetermined}.$$

Circular polarizations correspond to points on the equator:

$$|\mathrm{R}\rangle : \ \theta = \frac{\pi}{2}, \ \phi = \frac{\pi}{2}, \qquad |\mathrm{L}\rangle : \ \theta = \frac{\pi}{2}, \ \phi = -\frac{\pi}{2}.$$

https://doi.org/10.1017/CBO9780511755361.005

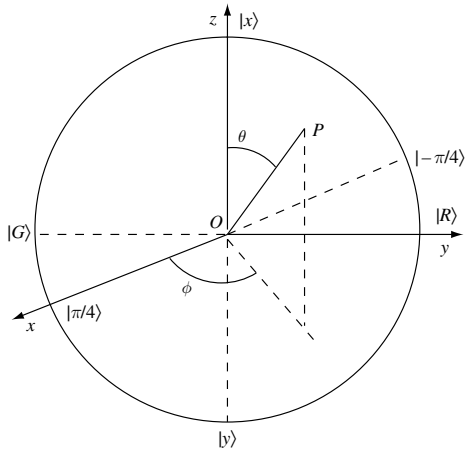

Figure 3.1 The Bloch sphere. The points on the Bloch sphere corresponding to the photon polarization bases $\{|x\rangle, |y\rangle\}$, $\{|R\rangle, |L\rangle\}$, and $\{|\theta = \pi/4\rangle, |\theta = -\pi/4\rangle\}$ are shown.

Another important physical realization of the qubit is spin 1/2. Let us introduce the subject by discussing a very well known phenomenon. A small magnetized needle is an approximate realization of what physicists call a *magnetic dipole*, characterized by a *magnetic dipole moment*, or simply *magnetic moment*, $\vec{\mu}$, which is an (axial) vector of $\mathbb{R}^3$. When placed in a magnetic field $\vec{B}$, this needle aligns itself in the direction of the field, just as the needle of a compass aligns itself with the Earth's magnetic field. The reason for this alignment is the following. The energy E of a magnetic dipole in a field $\vec{B}$ is

$$E = -\vec{\mu} \cdot \vec{B}, \tag{3.3}$$

and the minimum energy [1] is obtained when $\vec{\mu}$ is parallel to and in the same direction as $\vec{B}$. When the field is not uniform, the dipole moves toward the region where the field has the largest absolute value so as to minimize its energy. In summary, a dipole is subject to a torque which tends to align it with the field, and to a force which tends to make it move under the influence of a field *gradient*.

NMR (Nuclear Magnetic Resonance) and its derivative MRI (Imaging by (Nuclear) Magnetic Resonance [2]) are based on the fact that the proton [3] possesses a magnetic moment which can take two *and only two* values along the direction

[1] A physical system always struggles to reach a state of minimum energy (more correctly, minimum free energy).
[2] The adjective "nuclear" has been suppressed in order not to frighten the public...
[3] In fact, other nuclei of spin 1/2 such as ^{13}C, ^{19}F, and so on are also used in NMR; see Sec. 6.2. Only protons are used in MRI.

of a magnetic field. In other words, the component $\vec{\mu} \cdot \hat{n}$ of $\vec{\mu}$ along any axis $\hat{n}$ takes only two values, and this property characterizes a *spin 1/2 particle*. Experimentally, this can be seen as follows. A beam of protons[4] is sent into a magnetic field pointing in a direction $\hat{n}$ perpendicular to the beam direction. It is observed that the beam splits into two sub-beams, one deflected in the direction $\hat{n}$, and the other in the opposite direction $-\hat{n}$. This is the Stern–Gerlach experiment (Fig. 3.2, with $\hat{n} \parallel Oz$), which is in its principle a close analog of the separation of a ray of natural light into two rays by a birefringent crystal. The analog of a polarizer–analyzer experiment using spin 1/2 can also be imagined (Fig. 3.3). However, it should be noted that that the crossed polarizer–analyzer situation corresponds to

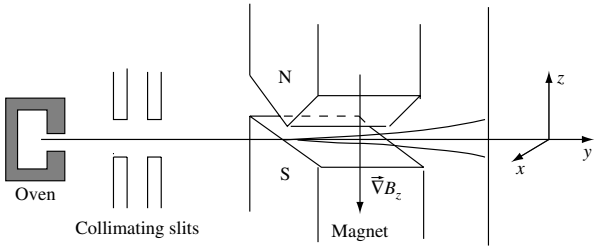

Figure 3.2 The Stern–Gerlach experiment. Silver atoms leaving an oven are collimated and pass through the gap of a magnet constructed such that the field is nonuniform with the gradient pointing in the $-z$ direction. It is actually the electron magnetic moment, which is a thousand times larger than the proton magnetic moment, which is responsible for the deflection.

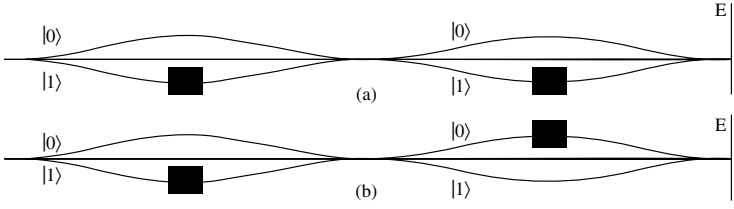

Figure 3.3 Crossed polarizers for spin 1/2. In case (a) 100% of the spins are transmitted by the second Stern–Gerlach apparatus, while 0% are transmitted in case (b). The two Stern–Gerlach filters select spin 1/2 particles in state $|0\rangle$ (upper beam) and state $|1\rangle$ (lower beam).

[4] This is a thought experiment. It is actually necessary to use neutral atoms rather than protons, as in Fig. 3.2; otherwise, the effects will be masked by forces due to the charges. Moreover, nuclear magnetism is too weak to be seen in such an experiment.

$\theta = \pi$ rather than $\theta = \pi/2$ as in the case of photons.[5] We construct a basis of $\mathcal{H}$ taking as the basis vectors $|0\rangle$ and $|1\rangle$, which correspond to states prepared by a magnetic field parallel to Oz. According to (3.1) and (3.2), the most general spin 1/2 state is

$$|\varphi\rangle = \mathrm{e}^{-\mathrm{i}\phi/2} \cos\frac{\theta}{2}|0\rangle + \mathrm{e}^{\mathrm{i}\phi/2} \sin\frac{\theta}{2}|1\rangle, \tag{3.4}$$

and it can be shown[6] that this state is the one selected by a magnetic field parallel to $\hat{n}$ with

$$\hat{n} = (\sin\theta\cos\phi, \sin\theta\sin\phi, \cos\theta). \tag{3.5}$$

In the spin 1/2 case, the Bloch sphere has an obvious geometrical interpretation: the spin 1/2 described by the vector (3.4) points in the direction $\hat{n}$.

We have seen that the physical properties of qubits are represented by Hermitian operators acting in a two-dimensional space. A convenient basis for these operators is that of the *Pauli matrices*:

$$\boxed{\sigma_1 (\text{or } \sigma_x) = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 (\text{or } \sigma_y) = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_3 (\text{or } \sigma_z) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}} \tag{3.6}$$

These matrices are Hermitian (and also unitary), and any 2×2 Hermitian matrix M can be written as

$$M = \lambda_0 I + \sum_{i=1}^{3} \lambda_i \sigma_i \tag{3.7}$$

with real coefficients. The Pauli matrices possess the following important properties:

$$\sigma_i^2 = I, \quad \sigma_1\sigma_2 = \mathrm{i}\sigma_3, \quad \sigma_2\sigma_3 = \mathrm{i}\sigma_1, \quad \sigma_3\sigma_1 = \mathrm{i}\sigma_2. \tag{3.8}$$

The states $|0\rangle$ and $|1\rangle$ are eigenvectors of σ_z with the eigenvalues ± 1:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{3.9}$$

and it can be verified immediately that the vector $|\varphi\rangle$ (3.4) is an eigenvector of

$$\vec{\sigma}\cdot\hat{n} = \sigma_x n_x + \sigma_y n_y + \sigma_z n_z = \begin{pmatrix} \cos\theta & \mathrm{e}^{-\mathrm{i}\phi}\sin\theta \\ \mathrm{e}^{\mathrm{i}\phi}\sin\theta & -\cos\theta \end{pmatrix} \tag{3.10}$$

[5] The photon has spin 1, and not 1/2! The rotation operator of a photon (Exercise 2.6.3) can be compared with that of a spin 1/2 (see Exercise 3.5.1), and it will be seen that it is the angle θ which arises in the first case and the angle $\theta/2$ in the second. A note for physicists: a massive particle of spin 1 possesses three polarization states, not two. An analysis performed by Wigner in 1939 shows that a zero-mass particle like the photon has only *two* polarization states no matter what its spin is.

[6] This is a consequence of the invariance under rotation; see Exercise 3.5.1.

https://doi.org/10.1017/CBO9780511755361.005

with eigenvalue $+1$. We also note that the vector $\langle\vec{\sigma}\rangle$, the expectation value of the spin in the state (3.4), is given by

$$\langle\vec{\sigma}\rangle = (\langle\sigma_x\rangle, \langle\sigma_y\rangle, \langle\sigma_x\rangle) \tag{3.11}$$

and points along $\hat{n}$.

We have just demonstrated the physical realization of a qubit by a spin 1/2, but there exist many other realizations, such as by a two-level atom, see the following section. In any case, the Hilbert space always has dimension 2, and the state of a qubit can always be represented by a point on the Bloch sphere.

3.2 Dynamical evolution

Now let us explicitly introduce the time, assuming that (3.1) holds at $t = 0$:

$$|\varphi(t=0)\rangle = \lambda(t=0)|0\rangle + \mu(t=0)|1\rangle, \qquad \lambda(t=0) = \lambda,\ \mu(t=0) = \mu. \tag{3.12}$$

Principle 3 We shall assume that the transformation

$$|\varphi(0)\rangle \to |\varphi(t)\rangle$$

is linear and that the norm of $|\varphi\rangle$ remains equal to one[7]

$$|\varphi(t)\rangle = \lambda(t)|0\rangle + \mu(t)|1\rangle, \tag{3.13}$$

$$|\lambda(t)|^2 + |\mu(t)|^2 = 1. \tag{3.14}$$

The transformation $|\varphi(0)\rangle \to |\varphi(t)\rangle$ is then a *unitary transformation* $U(t, 0)$ (a *unitary operator* U satisfies $U^{-1} = U^\dagger$; in a finite dimensional space, a linear operator which preserves the norm, called an isometry, is also a unitary operator):

$$|\varphi(t)\rangle = U(t, 0)|\varphi(t=0)\rangle.$$

In general,

$$|\varphi(t_2)\rangle = U(t_2, t_1)|\varphi(t_1)\rangle, \qquad U^\dagger(t_2, t_1) = U^{-1}(t_2, t_1). \tag{3.15}$$

Moreover, U must satisfy the group property:

$$U(t_2, t_1) = U(t_2, t')U(t', t_1), \tag{3.16}$$

[7] This second condition seems to be a natural consequence of state vector normalization, but in fact it involves the assumption that *all* the quantum degrees of freedom are included in $\mathcal{H}$: the evolution is not in general unitary when the qubit is only a part of a larger quantum system for which the Hilbert space of states is larger than $\mathcal{H}$, see Section 4.4.

https://doi.org/10.1017/CBO9780511755361.005

and, finally, $U(t,t) = I$. We use the group property and Taylor expansion for infinitesimal $\mathrm{d}t$ to write

$$U(t+\mathrm{d}t, t_0) = U(t+\mathrm{d}t, t)U(t, t_0),$$
$$U(t+\mathrm{d}t, t_0) \simeq U(t, t_0) + \mathrm{d}t\frac{\mathrm{d}}{\mathrm{d}t}U(t, t_0),$$
$$U(t+\mathrm{d}t, t)U(t, t_0) \simeq \left[I - \frac{\mathrm{i}}{\hbar}\mathrm{d}t\hat{H}(t)\right]U(t, t_0),$$

where we have defined the operator $\hat{H}(t)$, the *Hamiltonian*, as

$$\hat{H}(t) = \mathrm{i}\hbar\left.\frac{\mathrm{d}U(t', t)}{\mathrm{d}t'}\right|_{t'=t}. \tag{3.17}$$

The constant $\hbar = 1.05 \times 10^{-34}\,\mathrm{J\,s}$ was first introduced by Planck and is called Planck's constant. It relates energy E and frequency ω according to the *Planck–Einstein formula* $E = \hbar\omega$. The presence of the factor i ensures that $\hat{H}(t)$ is a Hermitian operator, while the presence of $\hbar$ implies that $\hat{H}$ has the dimension of an energy. In fact,

$$I = U^\dagger(t+\mathrm{d}t, t)U(t+\mathrm{d}t, t) \simeq \left[I + \frac{\mathrm{i}}{\hbar}\mathrm{d}t\hat{H}^\dagger(t)\right]\left[I - \frac{\mathrm{i}}{\hbar}\mathrm{d}t\hat{H}(t)\right]$$
$$\simeq I + \frac{\mathrm{i}}{\hbar}\mathrm{d}t(\hat{H}^\dagger - \hat{H}),$$

which implies that $\hat{H} = \hat{H}^\dagger$. From the above we see that the *evolution equation* (also called the *Schrödinger equation*) is

$$\boxed{\mathrm{i}\hbar\frac{\mathrm{d}U(t, t_0)}{\mathrm{d}t} = \hat{H}(t)U(t, t_0)} \tag{3.18}$$

Since $\hat{H}$ is a Hermitian operator, this is a physical property, and in fact $\hat{H}$ is just the *energy operator* of the system. In the often encountered case where the physics is invariant under time translation, the operator $U(t_2, t_1)$ depends only on the *difference* $(t_2 - t_1)$ and $\hat{H}$ is independent of time.

Let us illustrate this for the example of NMR (or MRI). In the first stage the spins 1/2 are placed in a strong, time independent magnetic field $\vec{B}_0$ (B_0 is a few teslas and 1 tesla $= 10^4$ gauss, about 10^4 times as strong as the Earth's magnetic field, which is why it is better not to wear one's watch when undergoing an MRI scan!). The Hamiltonian is then time independent, and since it is Hermitian it can be diagonalized in a certain basis:

$$\hat{H} = \begin{pmatrix} \hbar\omega_A & 0 \\ 0 & \hbar\omega_B \end{pmatrix}, \tag{3.19}$$

where $\hbar\omega_A$ and $\hbar\omega_B$ are the *energy levels* of the spin 1/2. If the magnetic field is parallel to Oz, the eigenvectors of $\hat{H}$ are just the basis vectors $|0\rangle$ and $|1\rangle$; see Box 3.1. Since $\hat{H}$ is independent of time, the evolution equation (3.18),

$$\mathrm{i}\hbar\frac{\mathrm{d}U}{\mathrm{d}t} = \hat{H}U,$$

can be integrated directly to give

$$U(t, t_0) = \exp[-\mathrm{i}\hat{H}(t - t_0)/\hbar], \tag{3.20}$$

or, in the basis in which $\hat{H}$ is diagonal,

$$U(t, t_0) = \begin{pmatrix} \mathrm{e}^{-\mathrm{i}\omega_A(t-t_0)} & 0 \\ 0 & \mathrm{e}^{-\mathrm{i}\omega_B(t-t_0)} \end{pmatrix}. \tag{3.21}$$

If $|\varphi(t = 0)\rangle$ is given by

$$|\varphi(t = 0)\rangle = \lambda|0\rangle + \mu|1\rangle,$$

then the state vector $|\varphi(t)\rangle$ at time t is

$$|\varphi(t)\rangle = \mathrm{e}^{-\mathrm{i}\omega_A t}\,\lambda|0\rangle + \mathrm{e}^{-\mathrm{i}\omega_B t}\,\mu|1\rangle \tag{3.22}$$

or

$$\lambda(t) = \mathrm{e}^{-\mathrm{i}\omega_A t}\,\lambda, \qquad \mu(t) = \mathrm{e}^{-\mathrm{i}\omega_B t}\,\mu.$$

The time evolution is *deterministic* and it keeps the memory of the initial conditions λ and μ. Owing to the arbitrariness of the phase, the only quantity which actually is physically relevant to the evolution is the difference

$$\omega_0 = \omega_B - \omega_A, \tag{3.23}$$

so that it is also possible to write $\hat{H}$ as

$$\hat{H} = -\frac{1}{2}\begin{pmatrix} \hbar\omega_0 & 0 \\ 0 & -\hbar\omega_0 \end{pmatrix}.$$

The quantity ω_0 plays an important role and is called the *resonance frequency*, and $\hbar\omega_0$ the *resonance energy*. By solving the equations of motion of a classical spin, it can be shown that the classical spin precesses about $\vec{B}_0$ with an angular frequency ω_0, the *Larmor frequency*.

Let us take this opportunity to mention another physical realization of a qubit, namely, a *two-level atom*. An atom possesses a large number of energy levels, but if we are interested in the effect of laser light on this atom, it is often possible to restrict ourselves to two particular levels, in general, the ground state ω_A and an excited state ω_B, $\omega_B > \omega_A$. This is referred to as the model of the two-level atom and it is very widely used in atomic physics. If the atom is raised to its

excited state, it returns spontaneously to its ground state by emitting a photon of frequency $\omega_0 = \omega_B - \omega_A$. If the atom in its ground state is hit with a laser beam of frequency $\omega \simeq \omega_0$, a *resonance phenomenon* is observed: the laser light will be absorbed more strongly the closer ω is to ω_0, a phenomenon which is analogous to that described in the following section in the case of spin 1/2.

3.3 Manipulating qubits: Rabi oscillations

Box 3.1: Interaction of a spin 1/2 with a magnetic field

An elementary calculation of classical physics shows that the magnetic moment $\vec{\mu}$ of a rotating charged system is proportional to its angular momentum $\vec{J}$, $\vec{\mu} = (\gamma/\hbar)\vec{J}$, where γ is called the *gyromagnetic ratio*. The proton spin is in fact an intrinsic angular momentum, rather as though the proton were spinning on its axis like a top. However, this classical image of the proton spin should be used with care, as it can be completely incorrect in the interpretation of certain phenomena; only a quantum description actually permits a real understanding of spin. Intrinsic angular momentum is a vectorial physical property with which there must be an associated Hermitian operator (more precisely, three Hermitian operators, one for each component). The proton spin is associated with the operator $\hbar\vec{\sigma}/2$. Note that the dimensionality is correct, because an angular momentum has the same dimension as $\hbar$. The magnetic moment, also a vector, is associated with a corresponding operator which must be proportional to the intrinsic angular momentum, because the only vector (actually, axial vector) at our disposal is $\vec{\sigma}$:

$$\vec{\mu} = \frac{1}{2}\gamma_p\vec{\sigma}, \qquad \gamma_p = 5.59\,\frac{q_p\hbar}{2m_p},$$

where γ_p is the gyromagnetic ratio of the proton, q_p is the proton charge, and m_p is the proton mass. The numerical value of γ_p must be taken from experiment,[8] and at present there is no reliable way to calculate it theoretically.[9]

As we shall see in Chapter 5, in quantum computing it is necessary to be able to transform a state, $|0\rangle$ for example, of a qubit into a linear superposition of $|0\rangle$ and $|1\rangle$. Taking spin 1/2 as an example, this can be done, as we shall see, by applying to the spin a constant magnetic field $\vec{B}_0$ parallel to Oz and a magnetic field $\vec{B}_1(t)$ rotating in the xOy plane with angular velocity ω:

$$\vec{B}_1(t) = B_1(\hat{x}\cos\omega t - \hat{y}\sin\omega t).$$

[8] The magnetic moment $\mu = 1.4 \times 10^{-28}$ J/T.

[9] In principle, it should be possible to calculate γ_p using the theory of strong interactions, QCD (Quantum ChromoDynamics). In practice, this calculation has to be done numerically (using lattice QCD), and the present accuracy is very far from permitting a good estimate of γ_p.

https://doi.org/10.1017/CBO9780511755361.005

The Hamiltonian of the proton magnetic moment in a magnetic field is written by analogy with (3.3), since $\hat{H}$ is the energy operator:

$$\hat{H} = -\vec{\mu}\cdot\vec{B} = -\frac{1}{2}\gamma_{\mathrm{p}}\vec{\sigma}\cdot\vec{B}.$$

The magnetic field used in NMR is

$$\vec{B} = B_0\hat{z} + B_1(\hat{x}\cos\omega t - \hat{y}\sin\omega t).$$

We define $\hbar\omega_0 = \gamma_{\mathrm{p}}B_0$ and $\hbar\omega_1 = \gamma_{\mathrm{p}}B_1$, and then the Hamiltonian becomes

$$\begin{aligned}\hat{H}(t) &= -\frac{1}{2}\gamma_{\mathrm{p}}B_0\sigma_z - \frac{1}{2}\gamma_{\mathrm{p}}B_1(\sigma_x\cos\omega t - \sigma_y\sin\omega t)\\ &= -\frac{\hbar}{2}\omega_0\sigma_z - \frac{\hbar}{2}\omega_1(\sigma_x\cos\omega t - \sigma_y\sin\omega t),\end{aligned}$$

and we find (3.24) using the explicit form (3.6) of the Pauli matrices. If $\vec{B}_1 = 0$, the Hamiltonian is time independent and its eigenvectors are $|0\rangle$ and $|1\rangle$, with eigenvalues $-\hbar\omega_0/2$ and $+\hbar\omega_0/2$, respectively.

Let a spin 1/2 be placed in a classical magnetic field with a periodic component as in Box 3.1:

$$\vec{B} = \vec{B}_0\hat{z} + B_1(\hat{x}\cos\omega t - \hat{y}\sin\omega t).$$

The form of $\hat{H}(t)$ then is (see Box 3.1 for the justification of (3.24))

$$\hat{H}(t) = -\frac{\hbar}{2}\begin{pmatrix}\omega_0 & \omega_1 e^{i\omega t}\\ \omega_1 e^{-i\omega t} & -\omega_0\end{pmatrix}, \tag{3.24}$$

where ω_1 is proportional to B_1 and can therefore be adjusted at will. The frequency ω_1 is called the *Rabi frequency*. The evolution equation (3.18) still needs to be solved. It is easily transformed into a system of two coupled first-order differential equations for $\lambda(t)$ and $\mu(t)$, which can be solved without difficulty (see Box 3.2 and Exercise 3.5.2). The result can be expressed as follows. If at time $t = 0$ the qubit is in the state $|0\rangle$, at time t it will have a probability $\mathsf{p}_{0\to1}(t)$ of being found in the state $|1\rangle$ given by

$$\mathsf{p}_{0\to1}(t) = \left(\frac{\omega_1}{\Omega}\right)^2\sin^2\frac{\Omega t}{2}, \qquad \Omega = \sqrt{(\omega-\omega_0)^2+\omega_1^2}. \tag{3.25}$$

https://doi.org/10.1017/CBO9780511755361.005

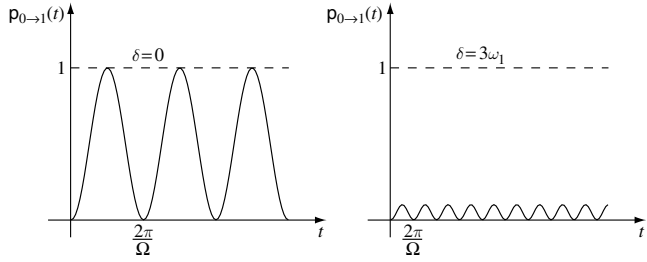

Figure 3.4 Rabi oscillations. The *detuning* δ is defined as $\delta = \omega - \omega_0$.

This is the phenomenon of *Rabi oscillations* (Fig. 3.4). The oscillation between the levels $|0\rangle$ and $|1\rangle$ has maximum amplitude for $\omega = \omega_0$, that is, at *resonance*:

$$p_{0\to1}(t) = \sin^2 \frac{\omega_1 t}{2}, \qquad \omega = \omega_0. \tag{3.26}$$

To go from the state $|0\rangle$ to the state $|1\rangle$ it is sufficient to adjust the time t during which the rotating field acts:

$$\frac{\omega_1 t}{2} = \frac{\pi}{2}, \qquad t = \frac{\pi}{\omega_1}.$$

This is called a π *pulse*. If a time intermediate between 0 and π/ω_1 is chosen, we obtain a superposition of $|0\rangle$ and $|1\rangle$. In particular, if $t = \pi/2\omega_1$ we have a $\pi/2$ *pulse*:

$$|0\rangle \to \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle). \tag{3.27}$$

This operation will be of crucial importance in quantum computing. The equations are essentially identical in the case of a two-level atom in the field of a laser when the generally well satisfied "rotating-wave approximation" is made. Then $\hbar\omega_0$ is the energy difference between the two atomic levels, ω is the frequency of the laser wave, and the Rabi frequency ω_1 is proportional to the product of the (transition) electric dipole moment of the atom $\vec{d}$ and the electric field $\vec{E}$ of the laser wave, $\omega_1 \propto \vec{d} \cdot \vec{E}\hbar$.

In summary, Rabi oscillations are the basic process used to manipulate qubits. These oscillations are obtained by exposing qubits to periodic electric or magnetic fields during suitably adjusted time intervals.

https://doi.org/10.1017/CBO9780511755361.005

Box 3.2: Solution of the NMR evolution equation at resonance

Equation (3.24) can immediately be transformed into an equation for $|\varphi(t)\rangle = U(t)|\varphi(t=0)\rangle$:

$$\mathrm{i}\hbar \frac{\mathrm{d}|\varphi(t)\rangle}{\mathrm{d}t} = \hat{H}(t)|\varphi(t)\rangle,$$

from which we find that $\lambda(t)$ and $\mu(t)$ obey a system of coupled differential equations:

$$\begin{aligned} \mathrm{i}\,\frac{\mathrm{d}\lambda(t)}{\mathrm{d}t} &= -\frac{\omega_0}{2}\lambda(t) - \frac{\omega_1}{2}\,\mathrm{e}^{\mathrm{i}\omega t}\,\mu(t), \\ \mathrm{i}\,\frac{\mathrm{d}\mu(t)}{\mathrm{d}t} &= -\frac{\omega_1}{2}\,\mathrm{e}^{-\mathrm{i}\omega t}\,\lambda(t) + \frac{\omega_0}{2}\mu(t). \end{aligned} \tag{3.28}$$

It is convenient to define

$$\lambda(t) = \hat{\lambda}(t)\mathrm{e}^{\mathrm{i}\omega_0 t/2}, \qquad \mu(t) = \hat{\mu}(t)\mathrm{e}^{-\mathrm{i}\omega_0 t/2}. \tag{3.29}$$

The system of differential equations simplifies to become

$$\begin{aligned} \mathrm{i}\,\frac{\mathrm{d}\hat{\lambda}(t)}{\mathrm{d}t} &= -\frac{\omega_1}{2}\,\mathrm{e}^{\mathrm{i}(\omega-\omega_0)t}\,\hat{\mu}(t), \\ \mathrm{i}\,\frac{\mathrm{d}\hat{\mu}(t)}{\mathrm{d}t} &= -\frac{\omega_1}{2}\,\mathrm{e}^{-\mathrm{i}(\omega-\omega_0)t}\,\hat{\lambda}(t). \end{aligned} \tag{3.30}$$

This system is easily transformed into a second-order differential equation for $\hat{\lambda}(t)$ (or $\hat{\mu}(t)$). Here we shall content ourselves with examining the case of resonance $\omega = \omega_0$ (see Exercise 3.5.2 for the general case), where

$$\frac{\mathrm{d}^2\hat{\lambda}(t)}{\mathrm{d}t^2} = -\frac{\omega_1^2}{4}\,\hat{\lambda}(t).$$

The solution of the system then is

$$\begin{aligned} \hat{\lambda}(t) &= a\cos\frac{\omega_1 t}{2} + b\sin\frac{\omega_1 t}{2}, \\ \hat{\mu}(t) &= \mathrm{i}a\sin\frac{\omega_1 t}{2} - \mathrm{i}b\cos\frac{\omega_1 t}{2}. \end{aligned} \tag{3.31}$$

The coefficients a and b depend on the initial conditions. Starting from, for example, the state $|0\rangle$ at time $t = 0$,

$$\lambda(t=0) = 1, \mu(t=0) = 0 \text{ or } a = 1,\ b = 0,$$

at time $t = \pi/2\omega_1$ (a $\pi/2$ pulse) we have a state which is a *linear superposition* of $|0\rangle$ and $|1\rangle$:

$$|\varphi(t)\rangle = \frac{1}{\sqrt{2}}\left(\mathrm{e}^{\mathrm{i}\omega_0 t/2}\,|0\rangle + \mathrm{i}\mathrm{e}^{-\mathrm{i}\omega_0 t/2}\,|1\rangle\right). \tag{3.32}$$

The phase factors can be absorbed by redefining the states $|0\rangle$ and $|1\rangle$ such that (3.27) is obtained.

https://doi.org/10.1017/CBO9780511755361.005

3.4 Principles of NMR and MRI

NMR spectroscopy is mainly used to determine the structure of complex chemical or biological molecules and for studying condensed matter in solid or liquid form. A detailed description of how NMR works would take us too far afield, and so we shall only touch upon the subject. The sample under study is placed in a uniform field $\vec{B}_0$ of several teslas, the maximum field accessible at present being about 20 T (Fig. 3.5). An NMR is characterized by the resonance frequency.[10] $\nu_0 = \omega_0/2\pi = \gamma_p B_0/(2\pi\hbar)$ for a proton: a field of 1 T corresponds to a frequency $\simeq 42.6$ MHz, and so we can speak of an NMR of 600 MHz if the field B_0 is 14 T. Owing to the Boltzmann law, the level $|0\rangle$ is more populated than the level $|1\rangle$, at least for $\gamma > 0$, which is the usual case. The ratio of the populations p_0 and p_1 at thermal equilibrium at absolute temperature T is, from the Boltzmann law,

$$\frac{\mathsf{p}_0(t=0)}{\mathsf{p}_1(t=0)} = \exp\left(\frac{\hbar\omega_0}{k_B T}\right), \tag{3.33}$$

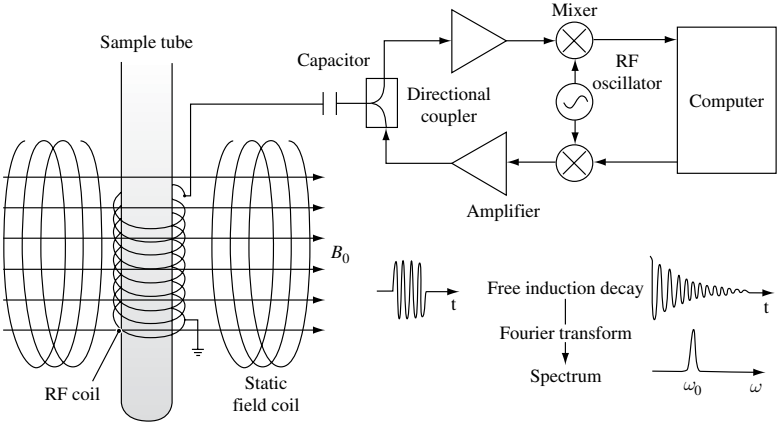

Figure 3.5 Schematics of the NMR principle. The static field $\vec{B}_0$ is horizontal and the radiofrequency field is generated by the vertical solenoid. This solenoid also serves as the signal detector (FID Free Induction Decay). The RF pulse and the signal are sketched at the lower right of the figure. The decreasing exponential form of the signal and the peak of its Fourier transform at $\omega = \omega_0$ should be noted. Adapted from Nielsen and Chuang (2000).

[10] More rigorously, ω is an *angular frequency*, measured in rad/s, whereas the *frequency* $\nu = \omega/2\pi$ is measured in Hz. Since we shall use ω almost exclusively, we shall refer to it somewhat casually as the frequency.

where k_B is the Boltzmann constant, $k_B = 1.38 \times 10^{-23}\,\mathrm{J/K}$. At the ambient temperature for an NMR of 600 MHz the population difference

$$\mathsf{p}_0 - \mathsf{p}_1 \simeq \frac{\hbar\omega_0}{2k_B T}$$

between the levels $|0\rangle$ and $|1\rangle$ is $\sim 5 \times 10^{-5}$.

The application at time $t = 0$ of a radiofrequency field $\vec{B}_1(t)$ during a time t such that $\omega_1 t = \pi$ with frequency ω_1 lying near the resonance frequency ω_0, that is, a π pulse, makes the spins of the state $|0\rangle$ go to the state $|1\rangle$ and vice versa, resulting in a *population inversion* with respect to the equilibrium populations, so that the sample is out of equilibrium. The return to equilibrium is characterized by a relaxation time [11] T_1, the *longitudinal relaxation time*. In practice, a $\pi/2$ pulse is used: $\omega_1 t = \pi/2$. This corresponds geometrically to rotating the spin by an angle $\pi/2$ about an axis of the xOy plane (Exercise 3.5.1). If the spin is initially parallel to $\vec{B}_0$, it ends up in a plane perpendicular to $\vec{B}_0$, a transverse plane (whereas a π pulse takes the spin to the longitudinal direction $-\vec{B}_0$). The return to equilibrium is then governed by a relaxation time T_2, the *transverse relaxation time*. The time T_1 is of the order of a second and $T_2 \lesssim T_1$; generally, $T_2 \ll T_1$. In any case, the return to equilibrium occurs with the emission of electromagnetic radiation of frequency $\simeq \omega_0$, and Fourier analysis of the signal gives a frequency spectrum which permits the structure of the molecule in question to be reconstructed. This is done on the basis of the following properties.

- The resonance frequency depends on the nuclei through γ.
- For a given nucleus the resonance frequency is slightly modified by the chemical environment of the atom to which the nucleus belongs, and this can be taken into account by defining an effective magnetic field B_0' acting on the nucleus:

$$B_0' = (1 - \sigma)B_0, \qquad \sigma \sim 10^{-6},$$

  where σ is called the *chemical shift*. There are strong correlations between σ and the nature of the chemical grouping to which the nucleus in question belongs.
- The interactions between neighboring nuclear spins provoke a splitting of the resonance frequencies into several subfrequencies which are also characteristic of the chemical groupings.

This is summarized in Fig. 3.6, where a typical NMR spectrum is given. It is important to observe that an NMR measurement has nothing to do with a projective measurement, as defined in Section 2.4. In fact, the NMR signal is a *collective* signal built up by spins located on $\sim 10^{18}$ molecules. When returning

[11] When a field $\vec{B}_0$ is applied, thermodynamical equilibrium (3.33) is not established instantaneously, but only after a time $\sim T_1$.

to equilibrium, these spins build up a a macroscopic polarization which precesses about the constant field $\vec{B}_0$. This precession induces an emf in a solenoid (the same solenoid which served to bring the spins to nonequilibrium), and this emf can be measured by standard methods. This gives rise to the free induction signal (FID) schematized in Fig. 3.5. This FID is Fourier analyzed, which allows one to determine the resonance frequencies, as in Fig. 3.6. The reason why the NMR measurement is a purely classical one is that spontaneous emission from a spin in an excited state, which must be described in a quantum framework, is completely negligible, so that the NMR measurement is best described in classical terms.

In the case of magnetic resonance imaging (MRI), it is only the protons contained in water and fats which are of interest. The sample is placed in a nonuniform field $\vec{B}_0$, which makes the resonance frequency depend on the spatial point. Since the signal amplitude is directly proportional to the spin density and therefore to the proton density, by complex computer calculations it is possible to deduce a three-dimensional image of the density of water in biological tissues. At present the spatial resolution is of the order of a millimeter, and an image can be made in 0.1 s. This has allowed the development of functional MRI (fMRI), which can be used, for example, to watch the brain in action by measuring local variations of the blood flow. The longitudinal and transverse relaxation times T_1 and T_2 play a major role in obtaining and interpreting MRI signals.

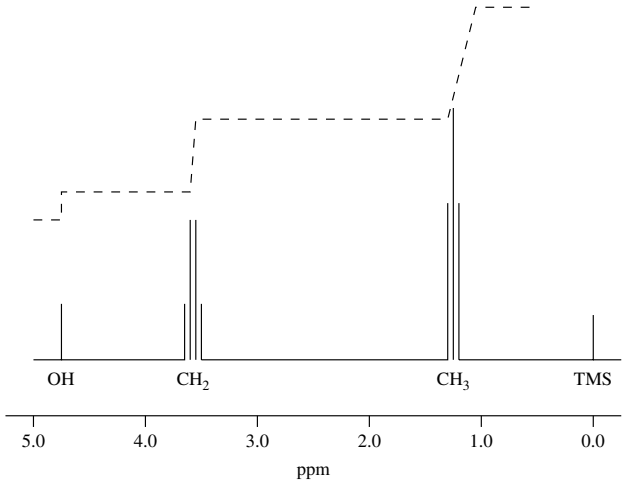

Figure 3.6 NMR spectrum of protons of ethanol CH_3CH_2OH obtained using an NMR of 200 MHz. The three peaks associated with the three groupings OH, CH_3, and CH_2 are clearly seen. The dashed line represents the integrated area of the signals. TMS (tetramethylsilane) is a reference signal.

3.5 Exercises

3.5.1 Rotation operator for spin 1/2

1. Show that the expectation value $\langle\vec{\sigma}\rangle$ of the operator $\vec{\sigma}$ in the state (3.4) is given by $\langle\vec{\sigma}\rangle = \hat{n}$, where $\hat{n}$ is defined in (3.11).
2. Show that

$$\exp\left(-\mathrm{i}\frac{\theta}{2}\,\vec{\sigma}\cdot\hat{p}\right) = I\cos\frac{\theta}{2} - \mathrm{i}(\vec{\sigma}\cdot\hat{p})\sin\frac{\theta}{2},$$

where $\hat{p}$ is a unit vector. Hint: calculate $(\vec{\sigma}\cdot\hat{p})^2$. The operator $\exp(-\mathrm{i}\theta\,\vec{\sigma}\cdot\hat{p}/2)$ is the unitary operator $U[\mathcal{R}_{\hat{p}}(\theta)]$ which rotates by an angle θ about the $\hat{p}$ axis. To see this, use the vector $\hat{p} = (-\sin\phi, \cos\phi, 0)$ as the rotation axis and show that a rotation by an angle θ about this axis takes the axis Oz to the vector $\hat{n}$ (3.5). Show that $\exp(-\mathrm{i}\theta\vec{\sigma}\cdot\hat{p}/2)|0\rangle$ is just the vector $|\varphi\rangle$ (3.4), the eigenvector of $\vec{\sigma}\cdot\hat{n}$ with eigenvalue $+1$ up to a global phase. What is $\exp(-\mathrm{i}\theta\,\vec{\sigma}\cdot\hat{p}/2)|1\rangle$?
3. When $\phi = -\pi/2$ the rotation is about Ox. Give the explicit matrix form of $U[\mathcal{R}_x(\theta)]$. Comparing with (3.31), show that under the action of $\vec{B}_1(t)$ the state vector rotates by an angle $\theta = -\omega_1 t$ if this field is applied during a time interval $[0, t]$.

3.5.2 Rabi oscillations away from resonance

1. In the nonresonant case, show that starting from (3.30) we obtain a second-order differential equation for $\hat{\lambda}(t)$:

$$\frac{2}{\omega_1}\frac{\mathrm{d}^2\hat{\lambda}}{\mathrm{d}t^2} - \frac{2\mathrm{i}}{\omega_1}\,\delta\,\frac{\mathrm{d}\hat{\lambda}}{\mathrm{d}t} + \frac{1}{2}\,\omega_1\hat{\lambda} = 0, \qquad \delta = \omega - \omega_0, \tag{3.34}$$

the solutions of which have the form

$$\hat{\lambda}(t) = \mathrm{e}^{\mathrm{i}\Omega_\pm t}.$$

Show that the values of $\Omega_\pm$ are the roots of a second-order equation and are given as a function of the frequency $\Omega = \left(\omega_1^2 + \delta^2\right)^{1/2}$ by

$$\Omega_\pm = \frac{1}{2}\Big[\delta \pm \Omega\Big].$$

2. The solution of (3.34) for $\hat{\lambda}$ is a linear combination of $\exp(\mathrm{i}\Omega_+ t)$ and $\exp(\mathrm{i}\Omega_- t)$:

$$\hat{\lambda}(t) = a\exp(\mathrm{i}\Omega_+ t) + b\exp(\mathrm{i}\Omega_- t).$$

Choose the initial conditions $\hat{\lambda}(0) = 1$, $\hat{\mu}(0) = 0$. Since $\hat{\mu}(0) \propto \mathrm{d}\hat{\lambda}(0)/\mathrm{d}t$, find a and b as functions of Ω and $\Omega_\pm$.

3. Show that the final result can be written as (see Exercise 6.5.1 for a more elegant proof of this result)

$$\hat{\lambda}(t) = \frac{e^{i\delta t/2}}{\Omega}\left[\Omega\cos\frac{\Omega t}{2} - i\delta\sin\frac{\Omega t}{2}\right],$$
$$\hat{\mu}(t) = \frac{i\omega_1}{\Omega}e^{-i\delta t/2}\sin\frac{\Omega t}{2},$$

which reduces to (3.31) when $\delta = 0$. Starting at $t = 0$ from the state $|0\rangle$, what is the probability of finding the spin in the state $|1\rangle$ at time t? Show that the maximum probability $\mathsf{p}_-^{\max}$ of making a transition from the state $|0\rangle$ to the state $|1\rangle$ for $\Omega t/2 = \pi/2$ is given by a *resonance curve* of width δ:

$$\mathsf{p}_-^{\max} = \frac{\omega_1^2}{\omega_1^2 + \delta^2} = \frac{\omega_1^2}{\omega_1^2 + (\omega - \omega_0)^2}.$$

Sketch the curve for $\mathsf{p}_-^{\max}$ as a function of ω. As shown in Fig. 3.4, the Rabi oscillations are maximal at resonance and decrease rapidly in amplitude with growing δ.

3.6 Further reading

The principles of quantum mechanics are discussed by, for example, Le Bellac (2006), Chapter 4, and Nielsen and Chuang (2000), Chapter 2. The Stern–Gerlach experiment is described in detail by Cohen-Tannoudji *et al.* (1977), Chapter IV, NMR and MRI by Levitt (2001).

https://doi.org/10.1017/CBO9780511755361.005