TWO STATE SYSTEMS

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1   Introduction

A two-state system does not just have two states! It has two *basis* states, namely the state space is a two-dimensional complex vector space. For such a state space the Hamiltonian can be viewed as the most general Hermitian 2×2 matrix. In the case when the Hamiltonian is time-independent, this Hermitian matrix is characterized by four real numbers.

Two-state systems are idealizations that are valid when other degrees of freedom are ignored. A spin one-half particle is a two-state system with regards to spin, but being a particle, it may move and thus has position, or momentum degrees of freedom that imply a much larger, higher dimensional state space. Only if we ignore these degrees of freedom – perhaps because the particle is at rest – we can speak of a two-state system.

We will study here two specific examples of two-state systems. The first will be the ammonia molecule, which exhibits curious oscillations. The second will be spin one-half particles as used in nuclear magnetic resonance.

The mathematics of two-state systems is always the same. In fact any two-state system can be visualized as a spin system, and this will sometimes be quite useful.

2 Spin precession in a magnetic field

Let us first recall our earlier discussion of magnetic dipole moments. Classically we had the following relation valid for a charged particle

$$\boldsymbol{\mu} \;=\; \frac{q}{2m}\mathbf{S} \tag{2.1}$$

where $\boldsymbol{\mu}$ is the dipole moment, q is the charge of the particle, m its mass, and $\mathbf{S}$ is its angular momentum, arising from its spinning. In the quantum world this equation gets modified by a constant unit-free factor g, different for each particle:

$$\boldsymbol{\mu} \;=\; g\,\frac{q}{2m}\mathbf{S} \;=\; g\frac{q\hbar}{2m}\frac{\mathbf{S}}{\hbar}\,. \tag{2.2}$$

Here $q\hbar/(2m)$ has the units of dipole moment. If we consider electrons and protons the following definitions are thus natural:

$$
\begin{aligned}
\text{Born magneton:} \quad \mu_B &= \frac{e\hbar}{2m_e} = 5.78 \times 10^{-11}\,\frac{\text{MeV}}{\text{Tesla}}\,, \\
\text{Nuclear magneton:} \quad \mu_N &= \frac{e\hbar}{2m_p} = 3.15 \times 10^{-14}\,\frac{\text{MeV}}{\text{Tesla}}\,.
\end{aligned}
\tag{2.3}
$$

Note that the nuclear magneton is about two-thousand times smaller than the Bohr magneton. Nuclear magnetic dipole moments are much smaller that that of the electron! Including the g constant we have the following results. For an electron $g = 2$ and since the electron charge is negative we get

$$\boldsymbol{\mu}_e \;=\; -2\,\mu_B\,\frac{\mathbf{S}}{\hbar}\,. \tag{2.4}$$

The dipole moment and the angular momentum are antiparallel. For a proton, the experimental result is

$$\boldsymbol{\mu}_p \;=\; 2.79\,\mu_N\,\frac{\mathbf{S}}{\hbar}\,. \tag{2.5}$$

The neutron is neutral, so one would expect no magnetic dipole moment. But the neutron is not elementary: it is made by electrically charged quarks. A dipole moment is thus possible, depending on the way quarks are distributed. Indeed, experimentally,

$$\boldsymbol{\mu}_n \;=\; -1.91\,\mu_N\,\frac{\mathbf{S}}{\hbar}\,. \tag{2.6}$$

Somehow the negative charge beats the positive charge in its contribution to the dipole moment of the neutron.

For notational convenience we introduce the constant γ from

$$\boxed{\;\boldsymbol{\mu} \;=\; \gamma\,\mathbf{S}\,, \quad \text{with} \;\; \gamma \;=\; \frac{gq}{2m}\,.\;} \tag{2.7}$$

If we insert the particle in a magnetic field $\mathbf{B}$, the Hamiltonian H_S for the spin system is

$$H_S \; = \; -\boldsymbol{\mu} \cdot \mathbf{B} \; = \; -\gamma \, \mathbf{B} \cdot \mathbf{S} \; = \; -\gamma \, (B_x \hat{S}_x + B_y \hat{S}_y + B_z \hat{S}_z) \, . \tag{2.8}$$

If, for example we have a magnetic field $\vec{B} = B\hat{z}$ along the z axis, the Hamiltonian is

$$H_S \; = \; -\gamma B \, \hat{S}_z \tag{2.9}$$

The associated time evolution unitary operator is

$$\mathcal{U}(t,0) \; = \; \exp\!\Big(-\frac{iH_S t}{\hbar}\Big) \; = \; \exp\!\Big(-\frac{i(-\gamma Bt)\hat{S}_z}{\hbar}\Big) \tag{2.10}$$

We now recall a result that was motivated in the homework. You examined a unitary operator $R_{\mathbf{n}}(\alpha)$ defined by a unit vector $\mathbf{n}$ and an angle α, and given by

$$R_{\mathbf{n}}(\alpha) \; = \; \exp\!\Big(-\frac{i\alpha \hat{S}_{\mathbf{n}}}{\hbar}\Big), \quad \text{with} \;\; \hat{S}_{\mathbf{n}} \equiv \mathbf{n} \cdot \mathbf{S} \, . \tag{2.11}$$

You found evidence that when acting on a spin state, this operator rotates it by an angle α about the axis defined by the vector $\mathbf{n}$. If we now compare (2.11) and (2.10) we conclude that $\mathcal{U}(t,0)$ should generate a rotation by the angle $(-\gamma Bt)$ about the z-axis. We now confirm this explicitly.

Consider a spin pointing at time equal zero along the direction specified by the angles (θ_0, ϕ_0):

$$|\Psi, 0\rangle \; = \; \cos\frac{\theta_0}{2}|+\rangle + \sin\frac{\theta_0}{2}e^{i\phi_0}|-\rangle \tag{2.12}$$

Given the Hamiltonian $H_S \; = \; -\gamma B \, \hat{S}_z$ in (2.9) we have

$$H_S|\pm\rangle \; = \; \mp\frac{\gamma B\hbar}{2} \, . \tag{2.13}$$

Then we have

$$\begin{aligned}
|\Psi, t\rangle \; &= \; e^{-iH_S t/\hbar}|\Psi, 0\rangle \; = \; e^{-iH_S t/\hbar}\Big(\cos\frac{\theta_0}{2}|+\rangle + \sin\frac{\theta_0}{2}e^{i\phi_0}|-\rangle\Big) \\
&= \; \cos\frac{\theta_0}{2}e^{-iH_S t/\hbar}|+\rangle + \sin\frac{\theta_0}{2}e^{i\phi_0}e^{-iH_S t/\hbar}|-\rangle \\
&= \; \cos\frac{\theta_0}{2}e^{+i\gamma Bt/2}|+\rangle + \sin\frac{\theta_0}{2}e^{i\phi_0}e^{-i\gamma Bt/2}|-\rangle
\end{aligned} \tag{2.14}$$

using (2.13). To recognize the resulting state it is convenient to factor out the phase that multiplies the $|+\rangle$ state:

$$|\Psi, t\rangle \; = \; e^{+i\gamma Bt/2}\Big(\cos\frac{\theta_0}{2}|+\rangle + \sin\frac{\theta_0}{2}e^{i(\phi_0-\gamma Bt)}|-\rangle\Big). \tag{2.15}$$

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Since the overall phase is not relevant we can now recognize the spin state as the state corresponding to the vector $\vec{n}(t)$ defined by angles

$$\begin{aligned}
\theta(t) &= \theta_0, \\
\phi(t) &= \phi_0 - \gamma Bt.
\end{aligned} \tag{2.16}$$

Keeping θ constant while changing ϕ indeed corresponds to a rotation about the z axis and, after time t, the spin has rotated an angle $(-\gamma Bt)$ as claimed above.

In fact spin states in a magnetic field precess in exactly the same way that magnetic dipoles in classical electromagnetism precess. The main fact from electromagnetic theory that we need is that in a magnetic field a dipole moment experiences a torque $\boldsymbol{\tau}$ given by

$$\boldsymbol{\tau} = \boldsymbol{\mu} \times \mathbf{B}. \tag{2.17}$$

Then the familiar mechanics equation for the rate of change of angular momentum being equal to the torque gives

$$\frac{d\mathbf{S}}{dt} = \boldsymbol{\tau} = \boldsymbol{\mu} \times \mathbf{B} = \gamma \mathbf{S} \times \mathbf{B}, \tag{2.18}$$

which we write as

$$\frac{d\mathbf{S}}{dt} = -\gamma \mathbf{B} \times \mathbf{S}. \tag{2.19}$$

We recognize that this equation states that the time dependent vector is rotating with angular velocity $\vec{\omega}_L$ given by

$$\boxed{\boldsymbol{\omega}_L = -\gamma \mathbf{B}.} \tag{2.20}$$

This is the so-called Larmor frequency. Indeed, this identification is standard in mechanics. A vector $\mathbf{v}$ rotating with angular velocity $\boldsymbol{\omega}$ satisfies the differential equation

$$\frac{d\mathbf{v}}{dt} = \boldsymbol{\omega} \times \mathbf{v}. \tag{2.21}$$

You can convince yourself of this with the help of a simple picture (see Figure 1). Also note that the differential equation shows that the derivative of $\mathbf{v}$, given by the right-hand side, is orthogonal to $\mathbf{v}$ because the cross product involves $\mathbf{v}$. This is as it should when the vector $\mathbf{v}$ is rotated. Indeed, show that the above differential equation implies that $\frac{d}{dt}\mathbf{v} \cdot \mathbf{v} = 0$, so that the length of $\mathbf{v}$ is unchanged.

The Hamiltonian of a general spin in a magnetic field (2.8) is then

$$\boxed{H_S = -\boldsymbol{\mu} \cdot \mathbf{B} = -\gamma \mathbf{B} \cdot \mathbf{S} = \boldsymbol{\omega}_L \cdot \mathbf{S}.} \tag{2.22}$$
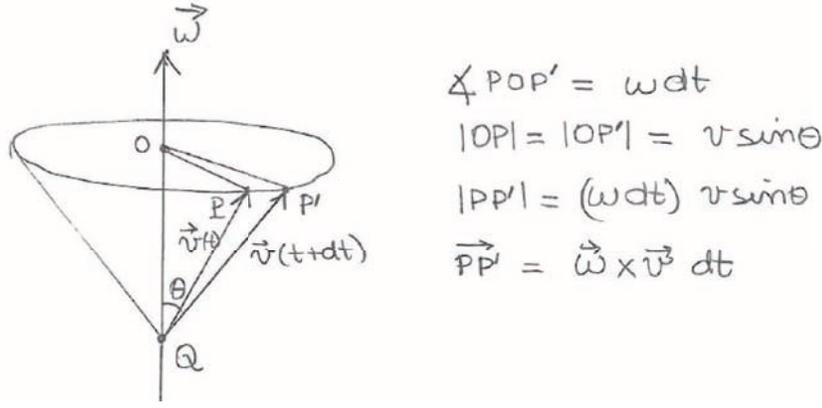
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Figure 1: The vector $\mathbf{v}(t)$ and an instant later the vector $\mathbf{v}(t + dt)$. The angular velocity vector $\boldsymbol{\omega}$ is along the axis and $\mathbf{v}$ rotates about is origin Q. At all times the vector $\mathbf{v}$ and $\boldsymbol{\omega}$ make an angle θ. The calculations to the right should convince you that (2.21) is correct.

For time independent magnetic fields $\boldsymbol{\omega}_L$ is also time independent and the evolution operator is

$$\mathcal{U}(t,0) \;=\; \exp\!\left(-iH_S t/\hbar\right) \;=\; \exp\!\left(-i\,\frac{\boldsymbol{\omega}_L \cdot \mathbf{S}}{\hbar}\,t\right). \tag{2.23}$$

If we write

$$\boldsymbol{\omega}_L \;=\; \omega_L\,\mathbf{n}, \quad \mathbf{n}\cdot\mathbf{n}=1, \tag{2.24}$$

we have

$$\mathcal{U}(t,0) \;=\; \exp\!\left(-i\,\frac{\omega_L t \hat{S}_\mathbf{n}}{\hbar}\right) \;=\; R_\mathbf{n}(\omega_L t), \tag{2.25}$$

where we compared with (2.11). The time evolution operator $\mathcal{U}(t,0)$ rotates the spin states by the angle $\omega_L t$ about the $\mathbf{n}$ axis. In other words

$$\boxed{\text{With } \; H_S \;=\; \boldsymbol{\omega}_L \cdot \mathbf{S} \; \text{ spin states precess with angular velocity } \; \boldsymbol{\omega}_L\,.} \tag{2.26}$$

3 The general two-state system viewed as a spin system

The most general time-independent Hamiltonian for a two-state system is a hermitian operator represented by the most general hermitian two-by-two matrix H. In doing so we are using some orthonomal basis $\{|1\rangle, |2\rangle\}$. In any such basis the matrix can be characterized by four real constants $g_0, g_1, g_2, g_3 \in \mathbb{R}$ as follows:

$$H \;=\; \begin{pmatrix} g_0 + g_3 & g_1 - ig_2 \\ g_1 + ig_2 & g_0 - g_3 \end{pmatrix} \;=\; g_0\mathbf{1} + g_1\sigma_1 + g_2\sigma_2 + g_3\sigma_3\,. \tag{3.27}$$

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On the right-hand side we wrote the matrix as a sum of matrices, where $\mathbf{1}$ and the Pauli matrices σ_i, $i = 1, 2, 3$ are hermitian. We view (g_1, g_2, g_3) as a vector $\mathbf{g}$ and then define

$$\mathbf{g} \cdot \boldsymbol{\sigma} \equiv g_1\sigma_2 + g_2\sigma_2 + g_3\sigma_3. \tag{3.28}$$

In this notation

$$\boxed{H = g_0\mathbf{1} + \mathbf{g} \cdot \boldsymbol{\sigma}.} \tag{3.29}$$

It is again convenient to introduce the magnitude g and the direction $\mathbf{n}$ of $\mathbf{g}$:

$$\mathbf{g} = g\,\mathbf{n}, \quad \mathbf{n} \cdot \mathbf{n} = 1, \quad g = \sqrt{g_1^2 + g_2^2 + g_3^2}. \tag{3.30}$$

Now the Hamiltonian reads

$$H = g_0\mathbf{1} + g\,\mathbf{n} \cdot \boldsymbol{\sigma}. \tag{3.31}$$

Recall now that the spin states $|\mathbf{n}; \pm\rangle$ are eigenstates of $\mathbf{n} \cdot \boldsymbol{\sigma}$

$$\mathbf{n} \cdot \boldsymbol{\sigma}\,|\mathbf{n}; \pm\rangle = \pm|\mathbf{n}; \pm\rangle. \tag{3.32}$$

In writing the spin states, however, you must recall that what we call the z-up and z-down states are just the first and second basis states: $|+\rangle = |1\rangle$ and $|-\rangle = |2\rangle$. With this noted, the spin states $|\mathbf{n}; \pm\rangle$ are indeed the eigenstates of H, since using the last two equations above we have

$$H|\mathbf{n}; \pm\rangle = (g_0 \pm g)|\mathbf{n}; \pm\rangle. \tag{3.33}$$

This also shows that the energy eigenvalues are $g_0 \pm g$. In summary:

$$\text{Spectrum:} \quad |\mathbf{n}; +\rangle \ \text{ with energy } g_0 + g, \quad |\mathbf{n}; -\rangle \ \text{ with energy } g_0 - g. \tag{3.34}$$

Thus our spin states allow us to write the general solution for the spectrum of the Hamiltonian (again, writing $|+\rangle = |1\rangle$ and $|-\rangle = |2\rangle$). Clearly the $|1\rangle$ and $|2\rangle$ states will generally have nothing to do with spin states. They are the basis states of any two-state system.

To understand the time evolution of states with the Hamiltonian H, we first rewrite H in terms of the spin operators, instead of the Pauli matrices, recalling that $\mathbf{S} = \frac{\hbar}{2}\boldsymbol{\sigma}$. Using (3.29) we find

$$H = g_0\mathbf{1} + \frac{2}{\hbar}\mathbf{g} \cdot \mathbf{S}. \tag{3.35}$$

Comparison with the spin Hamiltonian $H_S = \boldsymbol{\omega}_L \cdot \mathbf{S}$ shows that in the system described by H the states precess with angular velocity $\boldsymbol{\omega}$ given by

$$\boxed{\boldsymbol{\omega} = \frac{2}{\hbar}\,\mathbf{g}.} \tag{3.36}$$

Note that the part $g_0\mathbf{1}$ of the Hamiltonian H does not rotate states during time evolution; it simply multiplies states by the time-dependent phase $\exp(-ig_0t/\hbar)$.

Operationally, if H is known, the vector $\boldsymbol{\omega}$ above is immediately calculable. And given a normalized state $\alpha|1\rangle + \beta|2\rangle$ of the system ($|\alpha|^2 + |\beta|^2 = 1$), we can identify the corresponding spin state $|\mathbf{n}; +\rangle = \alpha|+\rangle + \beta|-\rangle$. The time evolution of the spin state is due to Larmor precession and is intuitively understood. With this result, the time evolution of the state in the original system is simply obtained by letting $|+\rangle \to |1\rangle$ and $|-\rangle \to |2\rangle$ in the precessing spin state.

4   The ammonia molecule as a two-state system

The ammonia molecule NH_3 is composed of four atoms, one nitrogen and three hydrogen. Ammonia is naturally a gas, without color, but with a pungent odor. It is mostly used for fertilizers, and also for cleaning products and pharmaceuticals.

The ammonia molecule takes the shape of a flattened tetrahedron. If we imagine the three hydrogen atoms forming an equilateral triangle at the base, the nitrogen atom sits atop. The angle formed between any two lines joining the nitrogen to the hydrogen is about $108°$ – this indeed corresponds to a flattened tetrahedron since a regular tetrahedron would have a $60°$ angle. If the nitrogen was pushed all the way down to the base, the angle would be $120°$.

The ammonia molecule has electronic excitations, vibrational excitations and rotational excitations. Those must largely be ignored in the two-state description of the molecule. The two states arise from transitions in which the nitrogen atom flips from being above the fixed hydrogen plane to being below the hydrogen plane. Since such a flip could be mimicked by a full rotation of the molecule, we can describe the transition more physically by considering the molecule spinning about the axis perpendicular to the hydrogen plane, with the N up, where up is the direction of the angular momentum. The transition would have the N down, or against the angular momentum of the rotating molecule.

More briefly, the two states are: nitrogen up, or nitrogen down. Both are classically stable configurations separated by a potential energy barrier. In classical mechanics these are the two options and they are degenerate in energy.

As long as the energy barrier is not infinite, in quantum mechanics the degeneracy is broken. This, of course is familiar. We can roughly represent the potential experienced by the nitrogen atom as the potential $V(z)$ in figure 3, where the two equilibrium positions of the nitrogen are at $\pm z_0$ and they are separated by a large barrier. In such a potential the ground state, which is symmetric, and the first excited state, which is antisymmetric, are almost degenerate in energy when the barrier is high. If the potential barrier was infinite, the two possible eigenstates would be the nitrogen wavefunction localized about z_0 and the nitrogen wavefunction localized about $-z_0$. Moreover, those states would be degenerate in energy. But with a large but finite barrier the ground state is represented by a wavefunction $\psi_g(z)$ even in z, as shown below the potential.
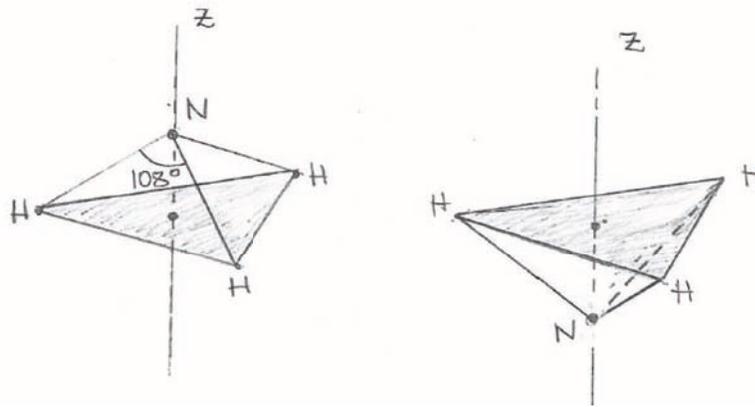
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Figure 2: The ammonia molecule looks like a flattened tetrahedron. The nitrogen atom can be up or down with respect to the plane defined by the three hydrogen atoms. These are the two states of the ammonia molecule.

This even wavefunction is roughly the superposition, with the same sign, of the two localized wavefunctions. The next excited state $\psi_e(z)$ is odd in z and is roughly the superposition, this time with opposite signs, of the two localized wavefunctions.
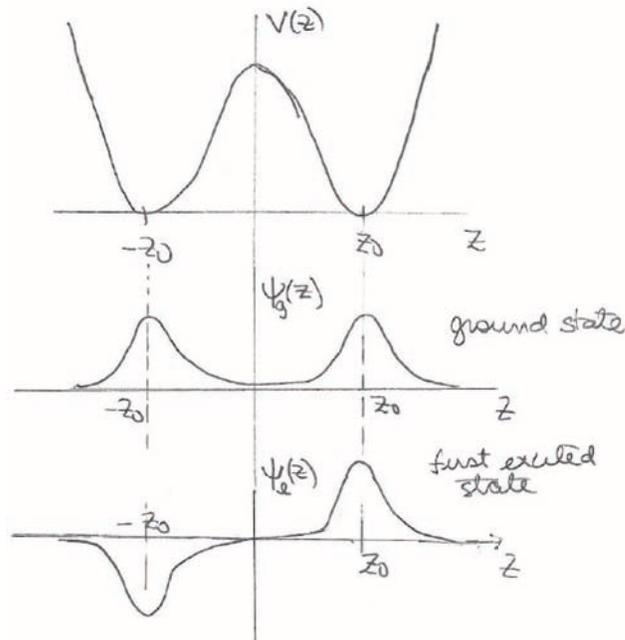

Figure 3: The potential $V(z)$ experienced by the nitrogen atom. There are two classically stable positions $\pm z_0$. The ground state and (first) excited state wavefunctions $\psi_g(z)$ and $\psi_e(z)$ are sketched below the potential.

Let us attempt a quantitative description of the situation. Let us label the two possible states:

$$|\uparrow\rangle \text{ is nitrogen up}, \qquad |\downarrow\rangle \text{ is nitrogen down} \tag{4.37}$$

We can associate to $|\uparrow\rangle$ a (positive) wavefunction localized around z_0 and to $|\downarrow\rangle$ a (positive) wavefunction localized around $-z_0$. Suppose the energy barrier is infinite. In this case the two states above must be energy eigenstates with the same energy E_0:

$$\begin{aligned} H|\uparrow\rangle &= E_0|\uparrow\rangle, \\ H|\downarrow\rangle &= E_0|\downarrow\rangle. \end{aligned} \tag{4.38}$$

The energy E_0 is arbitrary and will not play an important role. Choosing a basis

$$|1\rangle \equiv |\uparrow\rangle, \quad |2\rangle \equiv |\downarrow\rangle, \tag{4.39}$$

the Hamiltonian, in this basis takes the form of the two-by-two matrix

$$H = \begin{pmatrix} E_0 & 0 \\ 0 & E_0 \end{pmatrix}. \tag{4.40}$$

The ability to tunnel must correspond to off-diagonal elements in the Hamiltonian matrix – there is no other option, in fact! So we must have a nonzero $H_{12} = \langle 1|H|2\rangle \neq 0$. Since the Hamiltonian must be hermitian, we must have $H_{12} = H_{21}^*$. For the time being we will take the off-diagonal elements to be real and therefore:

$$H_{12} = H_{21} = -\Delta, \quad \Delta > 0. \tag{4.41}$$

The sign of the real constant Δ is conventional. We could change it by a change of basis in which we let, for example $|2\rangle \to -|2\rangle$. Our choice will be convenient. The full Hamiltonian is now

$$H = \begin{pmatrix} E_0 & -\Delta \\ -\Delta & E_0 \end{pmatrix} = E_0 \mathbf{1} - \Delta\sigma_1, \tag{4.42}$$

where in the last step we wrote the matrix as a sum of a real number times the two-by-two identity matrix plus another real number times the first Pauli matrix. Both the identity matrix and the Pauli matrix are hermitian, consistent with having a hermitian Hamiltonian. The eigenvalues of the Hamiltonian follow from the equation

$$\begin{vmatrix} E_0 - \lambda & -\Delta \\ -\Delta & E_0 - \lambda \end{vmatrix} = 0 \quad \to \quad (E_0 - \lambda)^2 = \Delta^2 \quad \to \quad \lambda_\pm = E_0 \pm \Delta. \tag{4.43}$$

The eigenstates corresponding to these eigenvalues are

$$\begin{aligned} |G\rangle &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle), \quad E = E_0 - \Delta, \text{ Ground state} \\ |E\rangle &= \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle), \quad E = E_0 + \Delta, \text{ Excited state} \end{aligned} \tag{4.44}$$

Here $|G\rangle$ is the ground state (thus the G) and $|E\rangle$ is the excited state (thus the E). Our sign choices make the correspondence of the states with the wavefunction in figure 3 clear. The ground state $|G\rangle$ is a superposition, with the same sign, of the two localized (positive) wavefunctions. The excited state $|E\rangle$ has the wavefunction localized at z_0 (corresponding to $|1\rangle$ with) a plus sign and the wavefunction localized at $-z_0$ (corresponding to $|2\rangle$) with at negative sign. Note that in the notation of section 3, the Hamiltonian in (4.42) corresponds to $\mathbf{g} = -\Delta\mathbf{x}$ and therefore $\mathbf{n} = -\mathbf{x}$ and $g = \Delta$. The excited state corresponds to the spin state $\frac{1}{\sqrt{2}}(|+\rangle - |-\rangle)$, which points in the $-\mathbf{x}$ direction. The ground state corresponds to the spin state $\frac{1}{\sqrt{2}}(|+\rangle + |-\rangle)$ which points in the $+\mathbf{x}$ direction.

The energy difference between these two eigenstates is 2Δ, which for the ammonia molecule takes the value

$$2\Delta = 0.9872 \times 10^{-4}\text{ev}. \tag{4.45}$$

Setting this energy equal to the energy of a photon that may be emitted in such a transition we find

$$2\Delta = \hbar\omega = h\nu, \quad \nu = 23.870 \times 10^{9}\text{Hz} = 23.870\,\text{GHz}, \tag{4.46}$$

corresponding to a wavelength λ of

$$\lambda = 1.2559\,\text{cm}. \tag{4.47}$$

Let us consider the time evolution of an ammonia molecule that at $t = 0$ is in the state $|\uparrow\rangle$. Using (4.44) we express the initial state in terms of energy eigenstates:

$$|\Psi, 0\rangle = |\uparrow\rangle = \frac{1}{\sqrt{2}}(|G\rangle + |E\rangle). \tag{4.48}$$

The time-evolved state can now be readily written:

$$|\Psi, t\rangle = \frac{1}{\sqrt{2}}\left(e^{-i(E-\Delta)t/\hbar}|G\rangle + e^{-i(E+\Delta)t/\hbar}|E\rangle\right), \tag{4.49}$$

and we now rewrite it in terms of the $|\uparrow\rangle, |\downarrow\rangle$ states as follows

$$\begin{aligned}
|\Psi, t\rangle &= \frac{1}{\sqrt{2}}\left(e^{-i(E-\Delta)t/\hbar}\frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) + e^{-i(E+\Delta)t/\hbar}\frac{1}{\sqrt{2}}(|\uparrow\rangle - |\downarrow\rangle)\right), \\
&= \frac{1}{2}e^{-iEt/\hbar}\left(e^{i\Delta t/\hbar}(|\uparrow\rangle + |\downarrow\rangle) + e^{-i\Delta t/\hbar}(|\uparrow\rangle - |\downarrow\rangle)\right), \\
&= e^{-iEt/\hbar}\left[\cos\left(\frac{\Delta t}{\hbar}\right)|\uparrow\rangle + i\sin\left(\frac{\Delta t}{\hbar}\right)|\downarrow\rangle\right].
\end{aligned} \tag{4.50}$$

The above time-dependent state oscillates from $|\uparrow\rangle$ to $|\downarrow\rangle$ with angular frequency $\omega = \Delta/\hbar \simeq$ 23 GHz. The probabilities $P_{\uparrow\downarrow}(t)$ that the state is found with nitrogen up or down are simply

$$\begin{aligned}
P_{\uparrow}(t) &= |\langle\uparrow|\Psi, t\rangle|^2 = \cos^2\left(\frac{\Delta t}{\hbar}\right), \\
P_{\downarrow}(t) &= |\langle\downarrow|\Psi, t\rangle|^2 = \sin^2\left(\frac{\Delta t}{\hbar}\right).
\end{aligned} \tag{4.51}$$

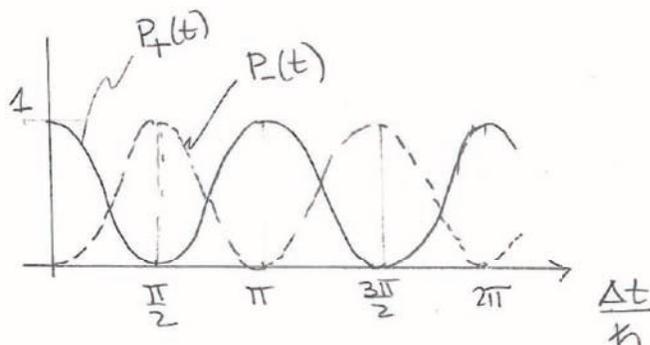A plot of these is shown in Figure 4

Figure 4: If the nitrogen atom starts in the state $| \uparrow \rangle$ at $t = 0$ (up position) then the probability $P_\uparrow(t)$ (shown as a continuous line) oscillates between one and zero. The probability $P_\downarrow(t)$ to be found in the state $| \downarrow \rangle$ is shown in dashed lines. Of course, $P_\uparrow(t) + P_\downarrow(t) = 1$. (Figure needs updating to change $\pm$ to $\uparrow\downarrow$.)

5 Ammonia molecule in an electric field

Let us now consider the electrostatic properties of the ammonia molecule. The electrons tend to cluster towards the nitrogen, leaving the nitrogen vertex slightly negative and the hydrogen plane slightly positive. As a result we get an electric dipole moment $\boldsymbol{\mu}$ that points down – when the nitrogen is up. The energy E of a dipole in an electric field $\boldsymbol{\mathcal{E}}$ is

$$E = -\boldsymbol{\mu} \cdot \boldsymbol{\mathcal{E}} . \tag{5.1}$$

With the electric field $\boldsymbol{\mathcal{E}} = \mathcal{E}\mathbf{z}$ along the z axis, and $\boldsymbol{\mu} = -\mu\mathbf{z}$, with $\mu > 0$, the state $| \uparrow \rangle$ with nitrogen up gets an extra positive contribution to the energy equal to $\mu\mathcal{E}$, while the $| \downarrow \rangle$ state gets the extra piece $-\mu\mathcal{E}$. The new Hamiltonian, including the effects of the electric field is then

$$H = \begin{pmatrix} E_0 + \mu\mathcal{E} & -\Delta \\ -\Delta & E_0 - \mu\mathcal{E} \end{pmatrix} = E_0 \mathbf{1} - \Delta \sigma_1 + \mu\mathcal{E} \sigma_3 , \tag{5.2}$$

This corresponds to $g = \sqrt{(\mu\mathcal{E})^2 + \Delta^2}$ and therefore the energy eigenvalues are

$$E_E(\mathcal{E}) = E_0 + \sqrt{\mu^2\mathcal{E}^2 + \Delta^2} ,$$
$$E_G(\mathcal{E}) = E_0 - \sqrt{\mu^2\mathcal{E}^2 + \Delta^2} , \tag{5.3}$$

where we added the subscripts E for excited and G for ground to identify the energies as those of the excited and ground states when $\mathcal{E} = 0$. For small $\mathcal{E}$, or more precisely, small $\mu\mathcal{E}/\Delta$, we

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have

$$E_E(\mathcal{E}) \simeq E_0 + \Delta + \frac{\mu^2 \mathcal{E}^2}{2\Delta} + \mathcal{O}(\mathcal{E}^4),$$

$$E_G(\mathcal{E}) \simeq E_0 - \Delta - \frac{\mu^2 \mathcal{E}^2}{2\Delta} + \mathcal{O}(\mathcal{E}^4),$$

(5.4)

while for large $\mu\mathcal{E}$

$$E_E(\mathcal{E}) \simeq E_0 + \mu\mathcal{E} + \mathcal{O}(1/\mathcal{E}),$$

$$E_G(\mathcal{E}) \simeq E_0 - \mu\mathcal{E} + \mathcal{O}(1/\mathcal{E}).$$

(5.5)

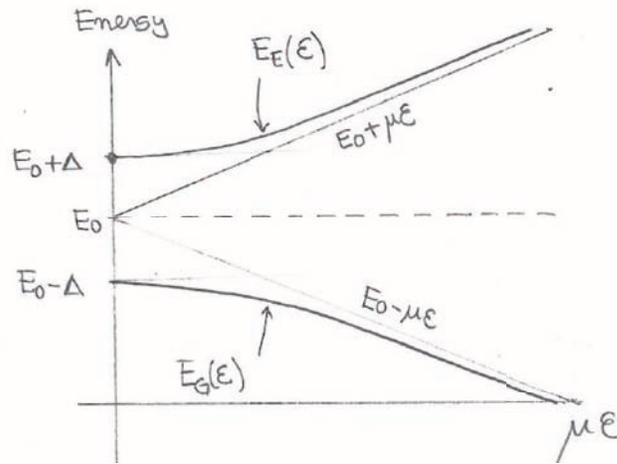A plot of the energies is shown in Figure 5.

Figure 5: The energy levels of the two states of the ammonia molecule as a function of the magnitude $\mathcal{E}$ of electric field. The higher energy state, with energy $E_E(\mathcal{E})$ coincides with $|E\rangle$ when $\mathcal{E} = 0$. The the lower energy state, with energy $E_G(\mathcal{E})$ coincides with $|G\rangle$ when $\mathcal{E} = 0$.

This analysis gives us a way to split a beam of ammonia molecules into two beams, one with molecules in the state $|G\rangle$ and one with molecules in the state $|E\rangle$. As shown in the figure we have a beam entering a region with a spatially dependent electric field. The electric field gradient points up: the magnitude of the field is larger above than below. In a practical device $\mu\mathcal{E} \ll \Delta$ and we can use (5.4). A molecule in the $|E\rangle$ state will tend to go to the region of lower $|\mathcal{E}$ as this is the region of low energy. Similarly a molecule in the $|G\rangle$ state will tend to go to the region of larger $|\mathcal{E}|$. Thus this device acts as a beam splitter.

The idea now is build a resonant electromagnetic cavity tuned to the frequency of 23.87 GHz and with very small losses (a high Q cavity). On one end, through a small hole, we let in a beam of ammonia molecules in the $|E\rangle$ state. These molecules exit the cavity through another
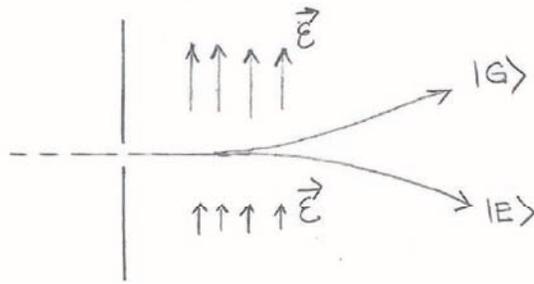
Figure 6: If a beam of ammonia molecules is exposed to an electric field with a strong gradient, molecules in the ground state $|G\rangle$ are deflected towards the stronger field (up) while molecules in the excited state $|E\rangle$ are deflected towards the weaker field (down).

hole on the opposite side (see Figure 7). If the design is done right, they exit on the ground state $|G\rangle$ thus having yielded an energy $2\Delta = \hbar\omega_0$ to the cavity. The ammonia molecules in the cavity interact with a spontaneously created electric field $\mathcal{E}$ that oscillates with the resonant frequency. The interaction with such field induces the transition $|E\rangle \to |G\rangle$. This transition also feeds energy into the field. We want to understand this transition.
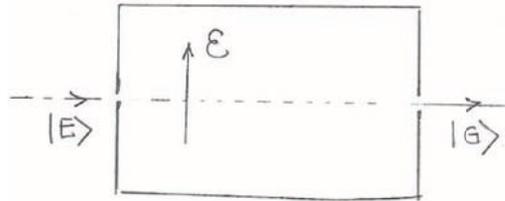

Figure 7: A resonant cavity tuned for 23.87GHz. A beam of ammonia molecules in the excited state $|E\rangle$ enter from the left. If properly designed, the molecules exit the cavity from the right on the ground state $|G\rangle$. In this process each molecule adds energy 2Δ to the electromagnetic field in the cavity.

The mathematics of the transition is clearer if we express the Hamiltonian in the primed basis

$$|1'\rangle \equiv |E\rangle, \quad |2'\rangle \equiv |G\rangle. \tag{5.6}$$

instead of the basis $|1\rangle = |\uparrow\rangle, |2\rangle = |\downarrow\rangle$ used to describe the Hamiltonian in (5.2). We can use

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(4.44) to calculate the new matrix elements. For example

$$
\begin{aligned}
\langle E|H|E\rangle &= \frac{1}{2}\big(\langle\uparrow| - \langle\downarrow|\big)H\big(|\uparrow\rangle - |\downarrow\rangle\big) \\
&= \frac{1}{2}\big(\langle\uparrow|H|\uparrow\rangle - \langle\uparrow|H|\downarrow\rangle - \langle\downarrow|H|\uparrow\rangle + \langle\downarrow|H|\downarrow\rangle\big) \\
&= \frac{1}{2}\big(E_0 + \mu\mathcal{E} - (-\Delta) - (-\Delta) + E_0 - \mu\mathcal{E}\big) \\
&= E_0 + \Delta\,,
\end{aligned}
\tag{5.7}
$$

and

$$
\begin{aligned}
\langle E|H|G\rangle &= \frac{1}{2}\big(\langle\uparrow| - \langle\downarrow|\big)H\big(|+\rangle + |\downarrow\rangle\big) \\
&= \frac{1}{2}\big(\langle+|H|\uparrow\rangle + \langle\uparrow|H|\downarrow\rangle - \langle\downarrow|H|\uparrow\rangle - \langle\downarrow|H|\downarrow\rangle\big) \\
&= \frac{1}{2}\big(E_0 + \mu\mathcal{E} + (-\Delta) - (-\Delta) - (E_0 - \mu\mathcal{E})\big) \\
&= \mu\mathcal{E}\,.
\end{aligned}
\tag{5.8}
$$

and similarly $\langle G|H|G\rangle = E_0 - \Delta$. All in all the Hamiltonian in the new basis is given by

$$
H = \begin{pmatrix} E_0 + \Delta & \mu\mathcal{E} \\ \mu\mathcal{E} & E_0 - \Delta \end{pmatrix} \quad \text{In the } |1'\rangle = |E\rangle,\ |2'\rangle = |G\rangle \text{ basis.}
\tag{5.9}
$$

We then write the wavefunction in terms of the amplitudes C_E and C_G to be in the $|E\rangle$ or $|G\rangle$ states respectively,

$$
|\Psi\rangle = \begin{pmatrix} C_E(t) \\ C_G(t) \end{pmatrix}.
\tag{5.10}
$$

The constant energy E_0 is not relevant – it can be set to any value and we choose the value zero. Doing so, the Schrödinger equation takes the form

$$
i\hbar\frac{d}{dt}\begin{pmatrix} C_E(t) \\ C_G(t) \end{pmatrix} = \begin{pmatrix} \Delta & \mu\mathcal{E} \\ \mu\mathcal{E} & -\Delta \end{pmatrix}\begin{pmatrix} C_E(t) \\ C_G(t) \end{pmatrix}.
\tag{5.11}
$$

A strategy to solve this equation is to imagine that $\mu\mathcal{E}$ is very small compared to Δ so that

$$
\begin{pmatrix} C_E(t) \\ C_G(t) \end{pmatrix} = \begin{pmatrix} e^{-i\Delta t/\hbar}\ \beta_E(t) \\ e^{+i\Delta t/\hbar}\ \beta_G(t) \end{pmatrix},
\tag{5.12}
$$

would be an exact solution with time-independent β_E and β_G if $\mu\mathcal{E} = 0$. When $\mu\mathcal{E}$ is small, we can expect solutions with β_E and β_G slowly varying in time (compared to the frequency $\Delta/\hbar$ of the phases we have brought out to the open. We now substitute into (5.11), with the result (do the algebra!) with several terms canceling and

$$
i\hbar\frac{d}{dt}\begin{pmatrix} \beta_E(t) \\ \beta_G(t) \end{pmatrix} = \begin{pmatrix} 0 & e^{i\omega_0 t}\mu\mathcal{E} \\ e^{-i\omega_0 t}\mu\mathcal{E} & 0 \end{pmatrix}\begin{pmatrix} \beta_E(t) \\ \beta_G(t) \end{pmatrix}, \quad \omega_0 \equiv \frac{2\Delta}{\hbar}
\tag{5.13}
$$

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where we defined ω_0 as the frequency of a photon associated to the transition $|E\rangle \to |G\rangle$. This frequency is the resonant frequency of the cavity to be used. We now assume that in the cavity the electric field $\mathcal{E}$ is at resonance so that

$$\mathcal{E}(t) \;=\; 2\mathcal{E}_0 \cos \omega_0 t \;=\; \mathcal{E}_0(e^{i\omega t} + e^{-i\omega t}) \tag{5.14}$$

so that

$$\begin{aligned} e^{i\omega_0 t} \mu \mathcal{E} &= \mu \mathcal{E}_0 (1 + e^{2i\omega_0 t}) \\ e^{-i\omega_0 t} \mu \mathcal{E} &= \mu \mathcal{E}_0 (1 + e^{-2i\omega_0 t}) \end{aligned} \tag{5.15}$$

We can now go back to the differential equation which gives

$$\begin{aligned} i\,\dot{\beta}_E(t) &= \frac{\mu \mathcal{E}_0}{\hbar}(1 + e^{2i\omega_0 t})\beta_G(t) \\ i\,\dot{\beta}_G(t) &= \frac{\mu \mathcal{E}_0}{\hbar}(1 + e^{-2i\omega_0 t})\beta_E(t)\,. \end{aligned} \tag{5.16}$$

With $\mu \mathcal{E}_0$ small, the rates of change of β_E and β_G will necessarily be small, as $\mu \mathcal{E}_0$ appears multiplicatively on the right-hand side. Thus β_E and β_G are essentially constant during the period of oscillation of the exponential terms $e^{\pm 2i\omega_0 t}$. Since these exponentials have zero time-averaged values, they can be dropped. Thus, we get

$$\begin{aligned} \dot{\beta}_E(t) &= -\,i\frac{\mu \mathcal{E}_0}{\hbar}\beta_G(t) \\ \dot{\beta}_G(t) &= -\,i\frac{\mu \mathcal{E}_0}{\hbar}\beta_E(t)\,. \end{aligned} \tag{5.17}$$

Taking another time derivative of the top equation we find;

$$\ddot{\beta}_E(t) \;=\; -\Big(\frac{\mu \mathcal{E}_0}{\hbar}\Big)^2 \beta_E(t) \tag{5.18}$$

This has the simple solution in terms of sines and cosines. If we assume that the molecule at time equal zero is indeed in the state $|E\rangle$ we then write

$$\beta_E(t) \;=\; \cos\Big(\frac{\mu \mathcal{E}_0}{\hbar}t\Big) \quad \to \quad \beta_G(t) \;=\; -i\sin\Big(\frac{\mu \mathcal{E}_0}{\hbar}t\Big)\,. \tag{5.19}$$

The time dependent probability $P_E(t)$ to be in the $|E\rangle$ state is then

$$P_E(t) = |C_E(t)|^2 \;=\; \big|e^{-i\Delta t/\hbar}\beta_E(t)\big| \;=\; \cos^2\Big(\frac{\mu \mathcal{E}_0}{\hbar}t\Big)\,. \tag{5.20}$$

This is our desired result. The molecule that enters the cavity in the state $|E\rangle$ will leave the cavity in the state $|G\rangle$ if the travel time T is such that the probability $P_E(T)$ to be in $|E\rangle$ vanishes. For this we need

$$\cos\Big(\frac{\mu \mathcal{E}_0}{\hbar}T\Big) \;=\; 0 \quad \to \quad \frac{\mu \mathcal{E}_0}{\hbar}T \;=\; \frac{\pi}{2}, \frac{3\pi}{2}, \dots\,. \tag{5.21}$$
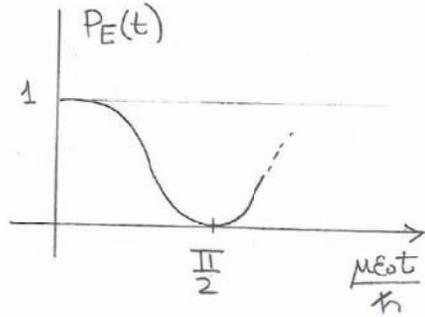
Figure 8: An ammonia molecule enters the resonant cavity at $t = 0$ in the excited state $|E\rangle$. We show probability $P_E(t)$ for the ammonia molecule to be in the excited $|E\rangle$ at time t. If the molecule exits at a time T for which $P_E(T) = 0$, the molecule will be in the ground state $|G\rangle$, as desired.

See figure 8.

If the velocity of the ammonia molecules is adjusted for this to happen, each molecule gives energy 2Δ to the cavity's electromagnetic field. The cavity's EM field, by producing the transition $|E\rangle \to |G\rangle$ of the traveling molecules, stimulates the emission of radiation. Moreover the energy released is in a field with the same configuration and frequency as the stimulating EM field. The molecules thus help build a *coherent* field in the cavity. Such a cavity is then a MASER, an acronym that stands for Microwave Amplification by Stimulated Emission of Radiation. The molecules are uncharged and therefore their motions produce no unwanted EM signals – this is in contrast to electrons in vacuum amplifiers, which produce *shot* noise.

Charles H. Townes, James P. Gordon, and H. J. Zeiger built the first ammonia maser working at Columbia University in 1953. As stated by Charles H. Townes in his Nobel lecture on December 11, 1964, "masers yield the most perfect amplification allowed by the uncertainty principle". For such EM waves the uncertainty principle can be written as

$$\Delta n \, \Delta \phi \geq \frac{1}{2},$$

where Δn is the uncertainty in the number of photons in the field and $\Delta \phi$ is the phase uncertainty of the wave, in radians. For a coherent field $\Delta n = \sqrt{\bar{n}}$, with $\bar{n}$ the expected number of photons. The saturation of the uncertainty principle leads to a phase uncertainty

$$\Delta \phi \;=\; \frac{1}{2\sqrt{\bar{n}}}, \tag{5.22}$$

that for any realistic $\bar{n}$ is fantastically small.

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6 Nuclear Magnetic Resonance

The problem we want to discuss is that of a spin in a time dependent magnetic field. This magnetic field has a time-independent z component and a circularly polarized field representing a magnetic field rotating on the (x, y) plane. More concretely, we have

$$\mathbf{B}(t) \; = \; B_0\,\mathbf{z} + B_1\big(\mathbf{x}\cos\omega t - \mathbf{y}\sin\omega t\big)\,. \tag{6.23}$$

Typically, the constant z-component B_0 is larger than B_1, the magnitude of the RF (radio-frequency) signal. The time dependent part of the field points along the x axis at $t = 0$ and is rotating with angular velocity ω in the clockwise direction of the (x, y) plane. The spin Hamiltonian is

$$H_S(t) \; = \; -\gamma\,\mathbf{B}(t)\cdot\mathbf{S} \; = \; -\gamma\Big(B_0\hat{S}_z + B_1\big(\cos\omega t\,\hat{S}_x - \sin\omega t\hat{S}_y\big)\Big)\,. \tag{6.24}$$

Not only is this Hamiltonian time dependent, but the Hamiltonian at different times do not commute. So this is a nontrivial time evolution problem!

We attempt to simplify the problem by considering a frame of reference that rotates with the magnetic field. For this, imagine first the case when $H_S = 0$ because the magnetic field is zero. With no magnetic field spin states would simply be static. What would the Hamiltonian be in the frame rotating about the z-axis with angular frequency ω, just like the magnetic field above? In that frame, the spin states that are fixed in the original frame would be seen to rotate with positive angular velocity ω about the z direction. There must be a Hamiltonian that does have that effect. Since the unitary operator $\mathcal{U}$ that generates this rotation is

$$\mathcal{U}(t) \; = \; \exp\Big(-\frac{i\omega t\hat{S}_z}{\hbar}\Big) \quad \to \quad H_{\mathcal{U}} \; = \; \omega\,\hat{S}_z\,, \tag{6.25}$$

where the expression $H_{\mathcal{U}}$ for the Hamiltonian in the rotating frame is read from the relation $\mathcal{U} = \exp(-iH_{\mathcal{U}}t/\hbar)$. For the original case, when the original Hamiltonian in the static frame is H_S, we will use the above operator $\mathcal{U}$ to define a new rotating-frame state $|\Psi_R\rangle$ as follows

$$|\Psi_R, t\rangle \; \equiv \; \mathcal{U}(t)|\Psi, t\rangle\,. \tag{6.26}$$

If we knew $|\Psi_R, t\rangle$ we would know $|\Psi, t\rangle$. We wish to find out if the Schrödinger equation for $|\Psi_R\rangle$ becomes simpler. For this we must determine the corresponding Hamiltonian H_R. One quick way to do this is to note that the above equation implies that

$$|\Psi_R, t\rangle \; \equiv \; \mathcal{U}(t)\mathcal{U}_S(t)|\Psi, 0\rangle\,. \tag{6.27}$$

where we have introduced the unitary operator $\mathcal{U}_S(t)$ associated with the Hamiltonian $H_S(t)$ that evolves $|\Psi\rangle$ in time. Since the Hamiltonian associated to an arbitrary unitary time-evolution operator $\mathcal{U}$ is $i\hbar(\partial_t\mathcal{U})\mathcal{U}^\dagger$ (if you don't recall this, derive it from a Schrödinger equation)

we have

$$
\begin{aligned}
H_R &= i\hbar\,\partial_t(\mathcal{U}\mathcal{U}_S)\,\mathcal{U}_S^\dagger\mathcal{U}^\dagger \\
&= i\hbar\,(\partial_t\mathcal{U})\mathcal{U}^\dagger + \mathcal{U}\,i\hbar\,(\partial_t\mathcal{U}_S)\mathcal{U}_S^\dagger\mathcal{U}^\dagger \\
\rightarrow \quad H_R &= H_\mathcal{U} + \mathcal{U}H_S\mathcal{U}^\dagger,
\end{aligned}
\tag{6.28}
$$

where $H_\mathcal{U}$ is the Hamiltonian associated to $\mathcal{U}$. Since $\mathcal{U}$ is the one above, we have $H_\mathcal{U} = \omega\hat{S}_z$ and therefore,

$$
\begin{aligned}
H_R &= \omega\hat{S}_z + \exp\!\left(-\frac{i\omega t\hat{S}_z}{\hbar}\right)\!\left[-\gamma\Big(B_0\hat{S}_z + B_1\big(\cos\omega t\,\hat{S}_x - \sin\omega t\hat{S}_y\big)\Big)\right]\exp\!\left(\frac{i\omega t\hat{S}_z}{\hbar}\right) \\
&= (-\gamma B_0 + \omega)\hat{S}_z - \gamma B_1\underbrace{\exp\!\left(-\frac{i\omega t\hat{S}_z}{\hbar}\right)\big(\cos\omega t\,\hat{S}_x - \sin\omega t\hat{S}_y\big)\exp\!\left(\frac{i\omega t\hat{S}_z}{\hbar}\right)}_{\hat{M}(t)}
\end{aligned}
\tag{6.29}
$$

and the big question is what is $\hat{M}(t)$. We can proceed by calculating the time-derivative of $\hat{M}$:

$$
\begin{aligned}
\partial_t\hat{M} &= e^{-\frac{i\omega t\hat{S}_z}{\hbar}}\left(-\frac{i\omega}{\hbar}\,\big[\hat{S}_z\,,\cos\omega t\,\hat{S}_x - \sin\omega t\hat{S}_y\big] + \big[-\omega\sin\omega t\,\hat{S}_x - \omega\cos\omega t\,\hat{S}_y\big]\right)e^{\frac{i\omega t\hat{S}_z}{\hbar}} \\
&= e^{-\frac{i\omega t\hat{S}_z}{\hbar}}\left(-\frac{i\omega}{\hbar}\,\big[i\hbar\cos\omega t\,\hat{S}_y + i\hbar\sin\omega t\hat{S}_x\big] + \big[-\omega\sin\omega t\,\hat{S}_x - \omega\cos\omega t\,\hat{S}_y\big]\right)e^{\frac{i\omega t\hat{S}_z}{\hbar}} \\
&= e^{-\frac{i\omega t\hat{S}_z}{\hbar}}\Big(\omega\cos\omega t\,\hat{S}_y + \omega\sin\omega t\hat{S}_x - \omega\sin\omega t\,\hat{S}_x - \omega\cos\omega t\,\hat{S}_y\Big)e^{\frac{i\omega t\hat{S}_z}{\hbar}} \\
&= 0\,.
\end{aligned}
\tag{6.30}
$$

This is very good news. Since $\hat{M}$ has no time dependence, we can evaluate it at any time. The simplest time is $t = 0$ and we thus find that

$$
\hat{M}(t) = \hat{S}_x\,.
\tag{6.31}
$$

As a result we have a totally time-independent H_R:

$$
\begin{aligned}
H_R &= (-\gamma B_0 + \omega)\hat{S}_z - \gamma B_1\hat{S}_x \\
&= -\gamma\left[\Big(B_0 - \frac{\omega}{\gamma}\Big)\hat{S}_z + B_1\hat{S}_x\right] \\
&= -\gamma\left[B_0\Big(1 - \frac{\omega}{\omega_0}\Big)\hat{S}_z + B_1\hat{S}_x\right],
\end{aligned}
\tag{6.32}
$$

using $\omega_0 = \gamma B_0$ for the Larmor frequency associated with the constant component of the field. We thus have a Hamiltonian H_R that can be associated with a magnetic field $\mathbf{B}_R$ given by Setting

$$
\boxed{\,H_R = -\gamma\,\mathbf{B}_R\cdot\mathbf{S}\,, \quad \rightarrow \quad \mathbf{B}_R = B_1\mathbf{x} + B_0\Big(1 - \frac{\omega}{\omega_0}\Big)\mathbf{z}\,.}
\tag{6.33}
$$

The full solution for the state is obtained beginning with (6.26) and (6.25):

$$|\Psi, t\rangle = \mathcal{U}^\dagger(t)|\Psi_R, t\rangle = \exp\left[\frac{i\omega t\hat{S}_z}{\hbar}\right]|\Psi_R, t\rangle. \tag{6.34}$$

Since H_R it a time-independent Hamiltonian, we have that the full time evolution is

$$|\Psi, t\rangle = \exp\left[\frac{i\omega t\hat{S}_z}{\hbar}\right] \exp\left[-i\frac{(-\gamma\mathbf{B}_R \cdot \mathbf{S})t}{\hbar}\right]|\Psi, 0\rangle \tag{6.35}$$

where the solution for $|\Psi_R, t\rangle$ is simply the time evolution from the $t = 0$ state generated by the Hamiltonian H_R. We have thus found that

$$\boxed{|\Psi, t\rangle = \exp\left[\frac{i\omega t\hat{S}_z}{\hbar}\right] \exp\left[i\frac{\gamma\mathbf{B}_R \cdot \mathbf{S}\,t}{\hbar}\right]|\Psi, 0\rangle.} \tag{6.36}$$

Exercise. Verify that for $B_1 = 0$ the above solution reduces to the one describing precession about the z-axis.

In the applications to be discussed below we always have

$$B_1 \ll B_0. \tag{6.37}$$

Consider now the evolution of a spin that initially points in the positive z direction. We look at two cases:

- $\omega \ll \omega_0$. In this case from (6.33) we have

$$\mathbf{B}_R \simeq B_0\mathbf{z} + B_1\mathbf{x}. \tag{6.38}$$

  This is a field mostly along the z axis, but tipped a little towards the x axis. The rightmost exponential in (6.36) makes the spin precess about the direction $\mathbf{B}_R$ quite quickly, for $|\mathbf{B}_R| \sim B_0$ and thus the angular rate of precession is pretty much ω_0. The next exponential in (6.36) induces a rotation about the z-axis with smaller angular velocity ω. This is shown in the figure.

- $\omega = \omega_0$. In this case from (6.33) we have

$$\mathbf{B}_R = B_1\mathbf{x}. \tag{6.39}$$

  In this case the right-most exponential in (6.36) makes the spin precess about the x axis it go from the z axis towards the y axis with angular velocity $\omega_1 = \gamma B_1$. If we time the RF signal to last a time T such that

$$\omega_1 T = \frac{\pi}{2} \quad \rightarrow \quad T = \frac{\pi}{2\gamma B_1}, \tag{6.40}$$

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the state $|\Psi_R, T\rangle$ points along the y axis. The effect of the other exponential in (6.36) is just to rotate the spin on the (x, y) plane. We have

$$|\Psi, t\rangle \;=\; \exp\Big[\frac{i\omega t \hat{S}_z}{\hbar}\Big]|\Psi_R, t\rangle\,, \quad t < T, \tag{6.41}$$

and if the RF pulse turns off after time T,

$$|\Psi, t\rangle \;=\; \exp\Big[\frac{i\omega t \hat{S}_z}{\hbar}\Big]|\Psi_R, T\rangle\,, \quad t > T, \tag{6.42}$$

The state $|\Psi, t\rangle$ can be visualized as a spin that is slowly rotating with angular velocity ω_1 from the z axis towards the plane, while rapidly rotating around the z axis with angular velocity ω. As a result the tip of the spin is performing a spiral motion on the surface of a hemisphere. By the time the polar angle reaches $\pi/2$ the RF signal turns off and the spin now just rotates within the (x, y) plane. This is called a 90° pulse.

Magnetic Resonance Imaging Based on work on nuclear magnetic resonance by Edward Purcell, who worked at MIT's radiation laboratory, and Felix Bloch. They got the Nobel prize for this work in 1952.

The NMR work led to the development of the technique called MRI for Magnetic Resonance Imaging. First studies in humans was done in 1977. The new perspective, as compared to X-rays, was that MRI allows one to distinguish various soft tissues.

The human body is mostly composed of water molecules. In those we have many hydrogen atoms, whose nuclei are protons and are the main players through their magnetic dipole moments (nuclear dipoles).

With a given external and large constant magnetic field B_0, at a given temperature, there is a net alignment of nuclear spins along B_0. This is called the "longitudinal magnetization". For all intents and purposes we have a net number of spins in play.

We apply a 90° pulse so that we get the spins to rotate with Larmor frequency ω_0 in the (x, y) plane. These rotating dipoles produce an oscillating magnetic field which is a signal that can be picked up by a receiver. The magnitude of the signal is proportional to the proton density. This is the first piece of information and allows differentiation of tissues.

The above signal from the rotation of the spins decays with a time constant T_2 that can be measured and is typically much smaller than a second. This decay is attributed to interactions between the spins. A T_2 weighted image allows doctors to detect abnormal accumulation of fluids (edema).

There is another time constant T_1 (of order one second) that controls the time to regain the longitudinal magnetization. This effect is due to the spins interacting with the rest of

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the lattice of atoms. White matter, grey matter, and cerebrospinal fluids are distinguished by different T_1 constants (they have about the same proton density).

MRI's commonly include the use of contrast agents, which are substances that shorten the time constant T_1 and are usually administered by injection into the blood stream. The contrast agent (gadolinium) can accumulate at organs or locations where information is valuable. For a number of substances one can use the MRI apparatus to determine their (T_1, T_2) constants and build a table of data. This table can then be used as an aid to identify the results of MRI's.

The typical MRI machine has a B_0 of about 2T (two tesla or 20,000 gauss). This requires a superconducting magnet with cooling by liquid helium. For people with claustrophobia there are "open" MRI scanners that work with lower magnetic fields. In addition there are about three *gradient* magnets, each of about 200 gauss. They change locally the value of B_0 and thus provide spatial resolution as the Larmor frequency becomes spatially dependent. One can thus attain spatial resolutions of about half a millimiter! MRI's are considered safe, as there is no evidence of biological harm caused by very large static magnetic fields.

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8.05 Quantum Physics II
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