

Nuclear Magnetic Resonance: Rabi's formula
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Rabi's frequency:

The **Rabi frequency** is the frequency of oscillation for a given atomic transition in a given light field. It is associated with the strength of the coupling between the light and the transition. Rabi flopping between the levels of a 2-level system illuminated with resonant light, will occur at the Rabi frequency. The Rabi frequency is a semi-classical concept as it is based on a quantum atomic transition and a classical light field. In the context of a nuclear magnetic resonance experiment, the Rabi frequency is the nutation frequency of a sample's net nuclear magnetization vector about a radiofrequency field. (Note that this is distinct from the Larmor frequency, which characterizes the precession of a transverse nuclear magnetization about a static magnetic field.)

http://en.wikipedia.org/wiki/Rabi_frequency

1. Proton magnetic moment

Proton magnetic moment is given by

$$\mu = \gamma I = \frac{g_N \mu_p}{\hbar} I = \frac{g_N \mu_p}{2} \sigma,$$

with

$$I = \frac{\hbar}{2} \sigma,$$

where I is a total angular momentum, $g_N (= 2)$ is the nuclear g factor, and γ is the gyromagnetic ratio,

$$\gamma = \frac{g_N \mu_p}{\hbar} = 2.67522 \times 10^4 \text{ [1/(s Oe)].}$$

μ_p is the nuclear magnetic moment,

$$\mu_p = 2.79270 \mu_N = 1.410606633 \times 10^{-23} \text{ emu,}$$

where μ_N is the nuclear magneton:

$$\mu_N = \frac{e\hbar}{2M_p c} = 5.05951 \times 10^{-24} \text{ emu.}$$

Here we use the notation for the magnetic moment of the proton as

$$\mu = \gamma \frac{\hbar}{2} \sigma = \mu_p \sigma,$$

with

$$\mu_p = \gamma \frac{\hbar}{2}.$$

2. Theory of NMR

The Hamiltonian with $\mathbf{B} = B_0 \mathbf{e}_z$

$$\hat{H}_0 = -\mu_z B_0 = -\gamma \frac{\hbar}{2} B_0 \hat{\sigma}_z,$$

$$\hat{H}_0 |\pm z\rangle = -\gamma \frac{\hbar}{2} B_0 \hat{\sigma}_z |\pm z\rangle = \mp \gamma \frac{\hbar}{2} B_0 |\pm z\rangle,$$

$$E_- - E_+ = \gamma \hbar B_0 = \hbar \omega_0,$$

$$f_0 \text{ (MHz)} = \omega_0 / 2\pi = 4.258 B_0 \text{ (kOe)},$$

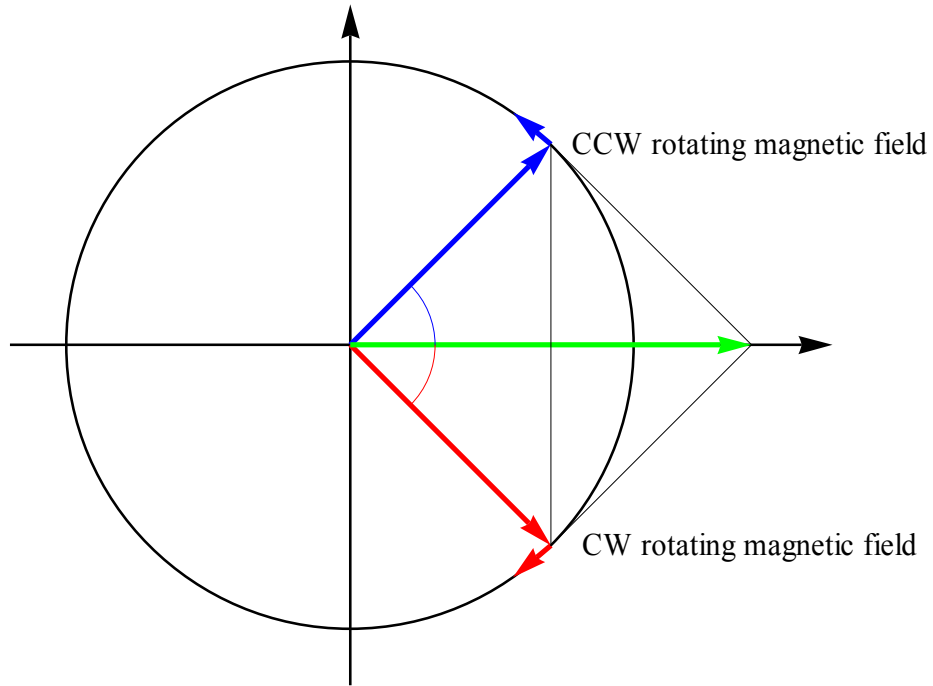
where γ is a gyromagnetic ratio; $\gamma = \frac{\mu_z}{I} = \frac{\mu_z}{\frac{\hbar}{2} \sigma_z}$.

Suppose that

$$\mathbf{B}_1 = 2 B_1 \cos(\omega t) \mathbf{e}_x, \quad (\text{linearly polarized})$$

is given by the superposition of counter-clockwise and clock-wise rotating magnetic fields,

$$\mathbf{B}_1 = [B_1 \cos(\omega t) \mathbf{e}_x + B_1 \sin(\omega t) \mathbf{e}_y] + [B_1 \cos(\omega t) \mathbf{e}_x - B_1 \sin(\omega t) \mathbf{e}_y].$$



Here we pick up the clock-wise rotating magnetic field,

$$\mathbf{B}_1 = B_1 \cos(\omega t)\mathbf{e}_x - B_1 \sin(\omega t)\mathbf{e}_y,$$

since the proton magnetic moment rotates around the z axis in a clockwise. The torque on the nuclear magnetic moment is given in the form such that

$$\boldsymbol{\mu} \times \mathbf{B}_0.$$

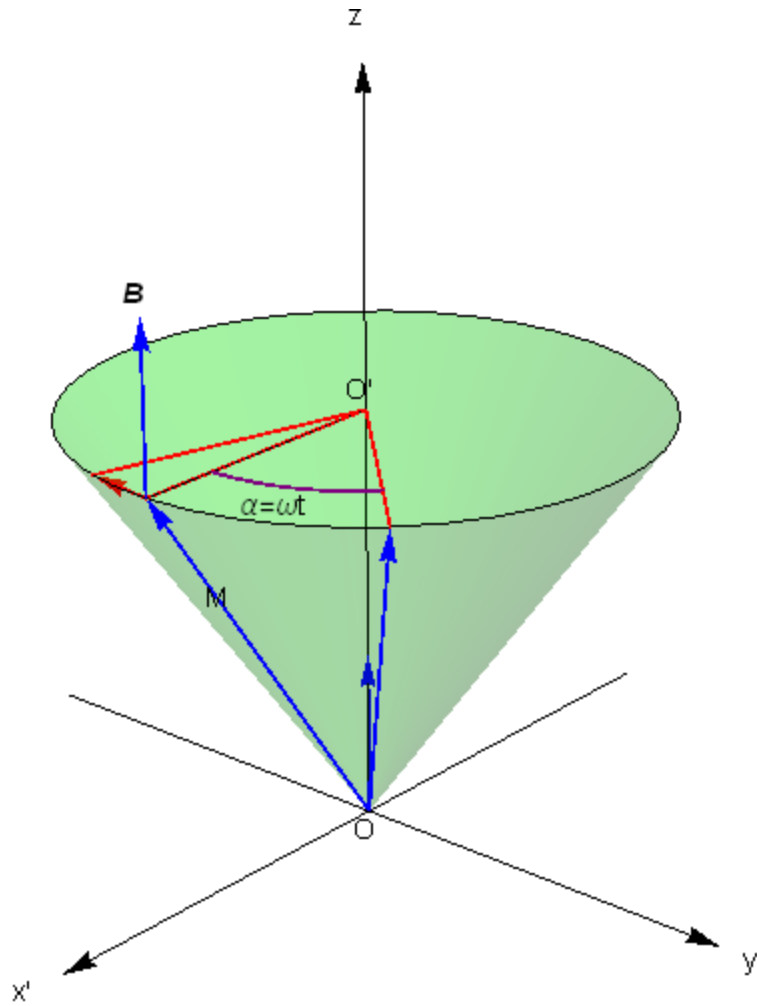


Fig. Larmor precession of the proton magnetic moment in the presence of an external magnetic field \mathbf{B}_0 along the z axis. The Larmor precession is done in the clockwise direction.

Then Hamiltonian \hat{H} is given by

$$\begin{aligned}
 \hat{H} &= -\hat{\boldsymbol{\mu}} \cdot \mathbf{B} \\
 &= -\gamma \frac{\hbar}{2} (\mathbf{B} \cdot \hat{\boldsymbol{\sigma}}) \\
 &= -\gamma \frac{\hbar}{2} [B_0 \hat{\sigma}_z + B_1 \cos(\omega t) \hat{\sigma}_x - B_1 \sin(\omega t) \hat{\sigma}_y]
 \end{aligned}$$

or

$$\hat{H} = -\gamma \frac{\hbar}{2} \begin{pmatrix} B_0 & B_1 e^{i\omega t} \\ B_1 e^{-i\omega t} & -B_0 \end{pmatrix},$$

where an external static magnetic field B_0 along the z axis and the rotating magnetic field $(B_1 \cos(\omega t), -B_1 \sin(\omega t), 0)$. Note that the Hamiltonian is dependent on the time t . We assume the wave function:

$$|\psi(t)\rangle = \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} = a_1(t)|+z\rangle + a_2(t)|-z\rangle.$$

We use the notations

$$\omega_0 = \gamma B_0, \quad \omega_1 = \gamma B_1,$$

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

under the basis of $\{|+z\rangle, |-z\rangle\}$. The state $|+z\rangle$ has energy $-\frac{1}{2}\hbar\omega_0$, and the state $|-z\rangle$ has energy $\frac{1}{2}\hbar\omega_0$. We therefore have a two-level system, the two Zeeman levels of a spin 1/2 in a magnetic field, with the energy difference of the levels being $\hbar\omega_0$.

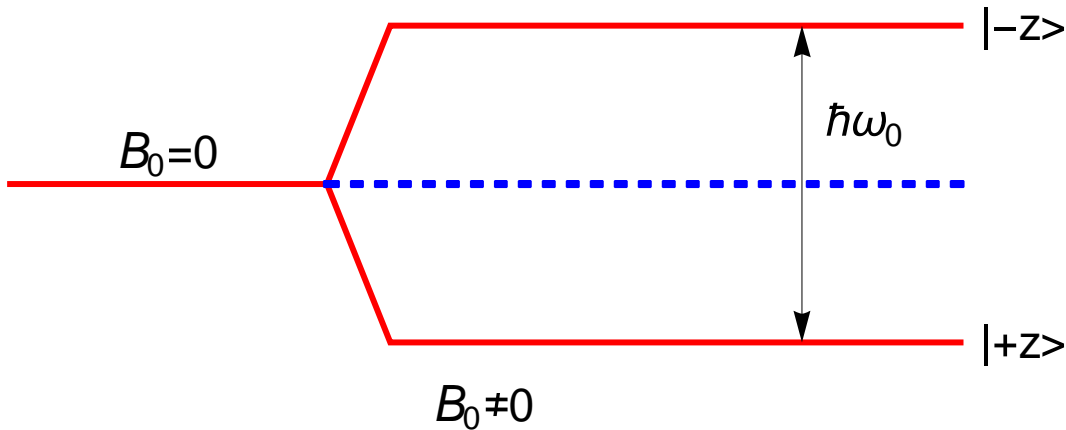


Fig. Zeeman splitting of the energy level with degenerate states (up and down spin states) in the presence of an external magnetic field.

The Schrödinger equation is given by

$$i\hbar \frac{\partial}{\partial t} |\psi(t)\rangle = i\hbar \begin{pmatrix} \frac{da_1}{dt} \\ \frac{da_2}{dt} \end{pmatrix} = \hat{H} \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} = -\gamma \frac{\hbar}{2} \begin{pmatrix} B_0 & B_1 e^{i\alpha t} \\ B_1 e^{-i\alpha t} & -B_0 \end{pmatrix} \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix},$$

or

$$\begin{pmatrix} \frac{da_1}{dt} \\ \frac{da_2}{dt} \end{pmatrix} = \frac{i}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{i\alpha t} \\ \omega_1 e^{-i\alpha t} & -\omega_0 \end{pmatrix} \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix}.$$

When $\omega_1 = 0$,

$$\begin{pmatrix} \frac{da_1}{dt} \\ \frac{da_2}{dt} \end{pmatrix} = \frac{i}{2} \begin{pmatrix} \omega_0 & 0 \\ 0 & -\omega_0 \end{pmatrix} \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix}.$$

Then we have

$$a_1(t) = e^{\frac{i\omega_0 t}{2}} a_1(0), \quad a_2(t) = e^{-\frac{i\omega_0 t}{2}} a_2(0).$$

For $\omega_1 \neq 0$, we assume that

$$a_1(t) = e^{\frac{i\omega_0 t}{2}} b_1(t), \quad a_2(t) = e^{-\frac{i\omega_0 t}{2}} b_2(t),$$

or

$$b_1(t) = e^{-\frac{i\omega_0 t}{2}} a_1(t), \quad b_2(t) = e^{\frac{i\omega_0 t}{2}} a_2(t),$$

where $b_1(t)$ and $b_2(t)$ are almost constant in the limit of $\omega_1 \rightarrow 0$, and equal to

$$b_1(t) \approx a_1(0), \quad b_2(t) \approx a_2(0).$$

((Definition of the new wave function)) Physical meaning

In order to solve the above differential equations, here we newly assume that

$$a_1(t) = e^{i\alpha t/2} b_1(t),$$

$$a_2(t) = e^{-i\omega t/2} b_2(t),$$

where we change $\omega_0 \rightarrow \omega$ in the above expressions.

((Laboratory frame and rotating reference frame))

We consider the rotation operator

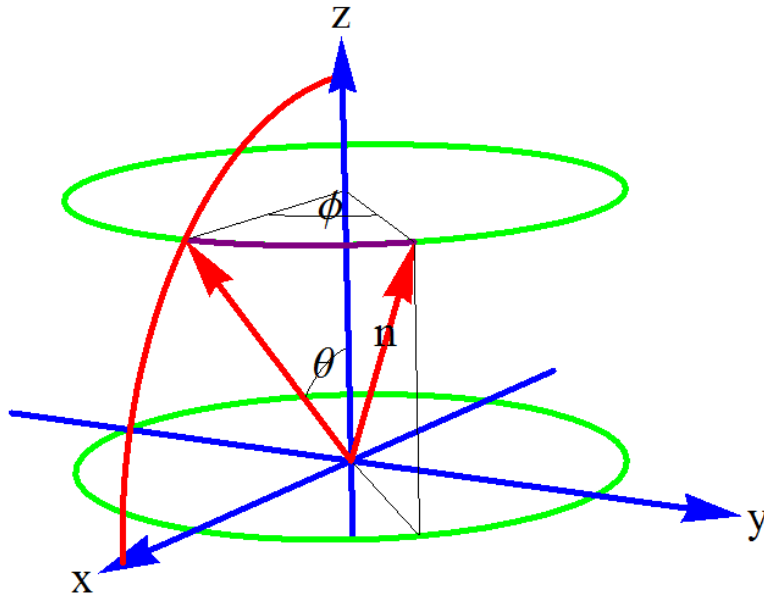
$$|\psi\rangle \rightarrow |\psi'\rangle = \hat{R}|\psi\rangle.$$

where $|\psi\rangle$ is the state vector in the laboratory frame and $|\psi'\rangle$ is the state vector in the rotating reference frame. \hat{R} is the rotation operator related to the geometrical rotation around the z axis in a counter clock wise, where

$$|\mathbf{r}'\rangle = |\mathfrak{R}\mathbf{r}\rangle = \hat{R}|\mathbf{r}\rangle \quad \text{for } \mathbf{r} \rightarrow \mathbf{r}' = \mathfrak{R}\mathbf{r}.$$

For the rotation around the z axis by an angle ϕ (in counter clock-wise), we have

$$\hat{R} = \exp\left(-\frac{i}{\hbar} \hat{J}_z \phi\right) = \exp\left(-\frac{i}{2} \hat{\sigma}_z \phi\right),$$



with

$$\phi = \omega t.$$

where ω is the angular frequency. Here we define the unitary operator (rotation operator) as

$$\hat{U}(t) = \hat{R} = \exp\left(-\frac{i}{2}\omega t \hat{\sigma}_z\right) = \begin{pmatrix} e^{-\frac{i}{2}\omega t} & 0 \\ 0 & e^{\frac{i}{2}\omega t} \end{pmatrix},$$

and

$$\hat{U}^\dagger(t) = \begin{pmatrix} e^{\frac{i}{2}\omega t} & 0 \\ 0 & e^{-\frac{i}{2}\omega t} \end{pmatrix}.$$

Note that

$$\hat{U}(t)|+z\rangle = \hat{R}|+z\rangle = \exp\left(-\frac{i}{2}\omega t \hat{\sigma}_z\right)|+z\rangle = e^{-\frac{i}{2}\omega t}|+z\rangle,$$

$$\hat{U}(t)|-z\rangle = \hat{R}|-z\rangle = \exp\left(-\frac{i}{2}\omega t \hat{\sigma}_z\right)|-z\rangle = e^{\frac{i}{2}\omega t}|-z\rangle.$$

We now consider the Schrödinger equation for $|\psi'(t)\rangle = \hat{U}(t)|\psi(t)\rangle$ (which is the state vector in the rotating reference frame),

$$\begin{aligned} |\psi'(t)\rangle &= \hat{U}(t)|\psi(t)\rangle \\ &= a_1(t)\hat{U}(t)|+z\rangle + a_2(t)\hat{U}(t)|-z\rangle \\ &= a_1(t)e^{-\frac{i}{2}\omega t}|+z\rangle + a_2(t)e^{\frac{i}{2}\omega t}|-z\rangle \\ &= b_1(t)|+z\rangle + b_2(t)|-z\rangle \\ &= \begin{pmatrix} b_1(t) \\ b_2(t) \end{pmatrix} \end{aligned}$$

and

$$\begin{pmatrix} b_1(t) \\ b_2(t) \end{pmatrix} = \begin{pmatrix} e^{-\frac{i}{2}\omega t} & 0 \\ 0 & e^{\frac{i}{2}\omega t} \end{pmatrix} \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix},$$

or

$$a_1(t) = e^{i\omega t/2} b_1(t),$$

$$a_2(t) = e^{-i\omega t/2} b_2(t).$$

Note that $b_1(t)$ and $b_2(t)$ are the components of the rotating reference frame, while $a_1(t)$ and $a_2(t)$ are the components of the laboratory frame.

Then we get

$$\frac{da_1(t)}{dt} = \frac{1}{2} e^{\frac{i}{2}\omega t} \left[i\omega b_1(t) + 2 \frac{db_1(t)}{dt} \right],$$

$$\frac{da_2(t)}{dt} = \frac{1}{2} e^{-\frac{i}{2}\omega t} \left[-i\omega b_2(t) + 2 \frac{db_2(t)}{dt} \right],$$

and

$$\begin{aligned} \frac{i}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{i\omega t} \\ \omega_1 e^{-i\omega t} & -\omega_0 \end{pmatrix} \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} &= \frac{i}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{i\omega t} \\ \omega_1 e^{-i\omega t} & -\omega_0 \end{pmatrix} \begin{pmatrix} e^{\frac{i}{2}\omega t} b_1(t) \\ e^{-\frac{i}{2}\omega t} b_2(t) \end{pmatrix} \\ &= \begin{pmatrix} \frac{i}{2} e^{\frac{i}{2}\omega t} [\omega_0 b_1(t) + \omega_1 b_2(t)] \\ \frac{i}{2} e^{-\frac{i}{2}\omega t} [\omega_1 b_1(t) - \omega_0 b_2(t)] \end{pmatrix} \end{aligned}$$

Thus we have

$$\begin{pmatrix} \frac{db_1}{dt} \\ \frac{db_2}{dt} \end{pmatrix} = \begin{pmatrix} \frac{i}{2}(\omega_0 - \omega) & \frac{i}{2}\omega_1 \\ \frac{i}{2}\omega_1 & -\frac{i}{2}(\omega_0 - \omega) \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}.$$

3. Solving differential equation

For simplicity we put

$$\Delta\omega = \omega_0 - \omega.$$

The Schrödinger equation can be rewritten as

$$i\hbar \begin{pmatrix} \frac{db_1}{dt} \\ \frac{db_2}{dt} \end{pmatrix} = \frac{\hbar}{2} \begin{pmatrix} \omega_0 - \omega & -\omega_1 \\ -\omega_1 & -(\omega_0 - \omega) \end{pmatrix} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix},$$

or

$$i\hbar \frac{d}{dt} |\psi'(t)\rangle = \hat{H}' |\psi'(t)\rangle,$$

where

$$\hat{H}' = \frac{\hbar}{2} \begin{pmatrix} \Delta\omega & -\omega_1 \\ -\omega_1 & -\Delta\omega \end{pmatrix},$$

and

$$|\psi'(t)\rangle = \begin{pmatrix} b_1(t) \\ b_2(t) \end{pmatrix},$$

under the basis of $\{|+z\rangle, |-z\rangle\}$. The solution of this equation is given by

$$|\psi'(t)\rangle = \exp\left(-\frac{i\hat{H}'t}{\hbar}\right) |\psi'(t=0)\rangle,$$

where \hat{H}' is independent of time t .

4. Eigenvalue problem

We can also solve the eigenvalue problem as follows. The Hamiltonian is given by

$$\hat{H}' = \frac{\hbar}{2} \begin{pmatrix} \Delta\omega & -\omega_1 \\ -\omega_1 & -\Delta\omega \end{pmatrix} = \frac{\hbar}{2} (\Delta\omega \hat{\sigma}_z - \omega_1 \hat{\sigma}_x).$$

This Hamiltonian indicates the Zeeman energy of spin in the presence of an effective magnetic field, which is expressed by

$$\mathbf{B}_{eff} = (B_0 - \frac{\omega}{\gamma})\mathbf{e}_z + (-B_1)\mathbf{e}_x = \frac{\omega_0 - \omega}{\gamma}\mathbf{e}_z + (-\frac{\omega_1}{\gamma})\mathbf{e}_x,$$

in the rotating reference frame.

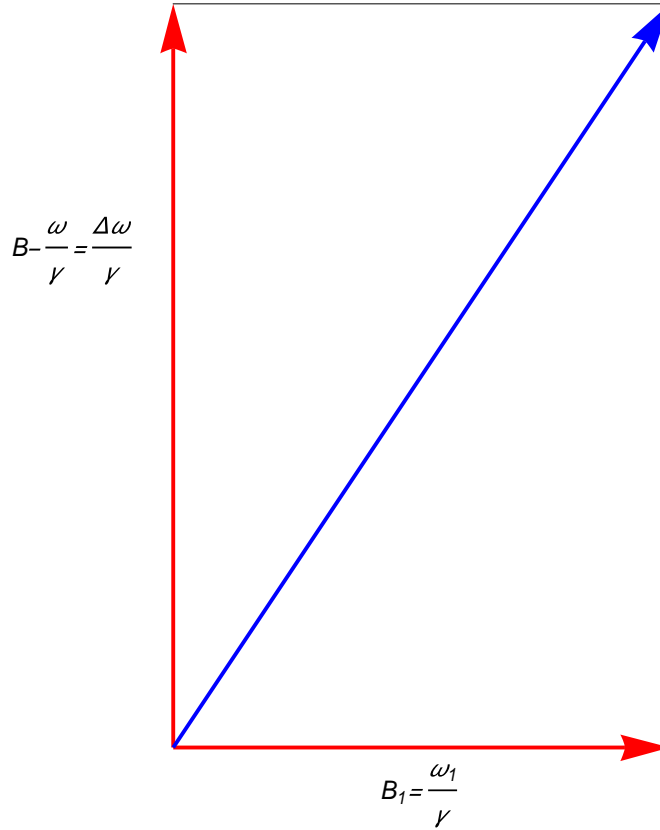


Fig. Effective magnetic field in the rotating reference frame.

or

$$\begin{aligned} \hat{H}' &= \frac{\hbar}{2} (\Delta\omega \hat{\sigma}_z - \omega_1 \hat{\sigma}_x) \\ &= -\frac{\hbar}{2} \sqrt{(\Delta\omega)^2 + \omega_1^2} \left(\frac{-\Delta\omega}{\sqrt{(\Delta\omega)^2 + \omega_1^2}} \hat{\sigma}_z + \frac{\omega_1}{\sqrt{(\Delta\omega)^2 + \omega_1^2}} \hat{\sigma}_x \right), \end{aligned}$$

or

$$\hat{H}' = -\frac{\hbar}{2} \sqrt{(\Delta\omega)^2 + \omega_1^2} (\hat{\sigma} \cdot \mathbf{n}),$$

where

$$(\hat{\sigma} \cdot \mathbf{n}) |\pm \mathbf{n}\rangle = \pm |\pm \mathbf{n}\rangle,$$

or

$$\begin{aligned}\hat{H}'|\pm \mathbf{n}\rangle &= -\frac{\hbar}{2}\sqrt{(\Delta\omega)^2 + \omega_1^2}(\hat{\sigma} \cdot \mathbf{n})|\pm \mathbf{n}\rangle \\ &= \mp \frac{\hbar}{2}\sqrt{(\Delta\omega)^2 + \omega_1^2}|\pm \mathbf{n}\rangle\end{aligned}$$

Thus $|\pm \mathbf{n}\rangle$ is the eigenket of \hat{H}' with the eigenvalues $\mp E$ with

$$E = \frac{\hbar\Omega}{2},$$

with

$$\Omega = \sqrt{(\Delta\omega)^2 + \omega_1^2},$$

$$|+\mathbf{n}\rangle = \cos\frac{\theta}{2}|+z\rangle + \sin\frac{\theta}{2}| -z\rangle,$$

$$|-\mathbf{n}\rangle = -\sin\frac{\theta}{2}|+z\rangle + \cos\frac{\theta}{2}| -z\rangle,$$

where

$$\cos\theta = \frac{-\Delta\omega}{\sqrt{(\Delta\omega)^2 + \omega_1^2}}, \quad \sin\theta = \frac{\omega_1}{\sqrt{(\Delta\omega)^2 + \omega_1^2}},$$

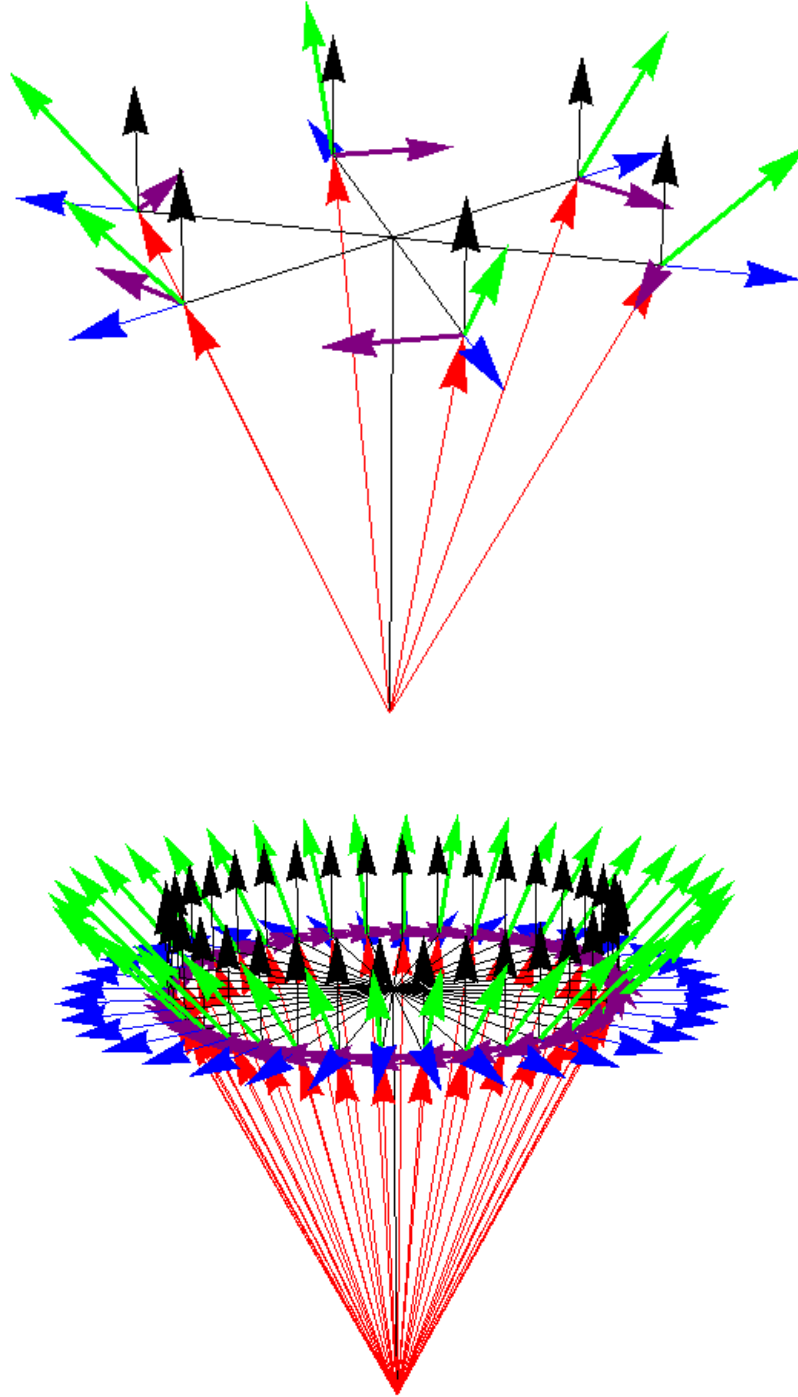


Fig. Red arrow (the nuclear magnetization). Blue arrow (rf magnetic field). Black arrow (the effective magnetic field along the z axis). Green arrow (the resultant effective magnetic field). The purple arrow (the torque).

5. Rabi's formula

We assume that the initial condition is given by

$$|\psi'(t=0)\rangle = |\psi(t=0)\rangle = |+z\rangle, \quad (\text{initial condition})$$

$$\begin{aligned} \exp\left(-\frac{i\hat{H}'t}{\hbar}\right) &= \exp\left(-\frac{i\hat{H}'t}{\hbar}\right)(|+n\rangle\langle+n| + |-n\rangle\langle-n|) \\ &= \exp\left(-\frac{i\hat{H}'t}{\hbar}\right)|+n\rangle\langle+n| + \exp\left(-\frac{i\hat{H}'t}{\hbar}\right)|-n\rangle\langle-n| \\ &= \exp\left(\frac{i\Omega t}{2}\right)|+n\rangle\langle+n| + \exp\left(-\frac{i\Omega t}{2}\right)|-n\rangle\langle-n| \end{aligned}$$

$$\begin{aligned} |\psi'(t)\rangle &= \exp\left(-\frac{i\hat{H}'t}{\hbar}\right)|+z\rangle \\ &= \exp\left(\frac{i\Omega t}{2}\right)|+n\rangle\langle+n| + z\rangle + \exp\left(-\frac{i\Omega t}{2}\right)|-n\rangle\langle-n| + z\rangle \\ &= \exp\left(i\frac{\Omega}{2}t\right)\cos\left(\frac{\theta}{2}\right)|+n\rangle - \sin\left(\frac{\theta}{2}\right)\exp\left(-i\frac{\Omega}{2}t\right)|-n\rangle \end{aligned}$$

or

$$\begin{aligned} \langle -z|\psi'(t)\rangle &= \exp\left(i\frac{\Omega}{2}t\right)\cos\left(\frac{\theta}{2}\right)\langle -z|+n\rangle - \sin\left(\frac{\theta}{2}\right)\exp\left(-i\frac{\Omega}{2}t\right)\langle -z|-n\rangle \\ &= \cos\left(\frac{\theta}{2}\right)\sin\left(\frac{\theta}{2}\right)\left[\exp\left(i\frac{\Omega}{2}t\right) - \exp\left(-i\frac{\Omega}{2}t\right)\right] \\ &= i\sin\theta\sin\left(\frac{\Omega}{2}t\right) \\ &= i\sin\theta\sin\left(\frac{t}{2}\sqrt{(\Delta\omega)^2 + \omega_1^2}\right) \end{aligned}$$

$$\begin{aligned} \langle +z|\psi'(t)\rangle &= \exp\left(i\frac{\Omega}{2}t\right)\cos\left(\frac{\theta}{2}\right)\langle +z|+n\rangle - \sin\left(\frac{\theta}{2}\right)\exp\left(-i\frac{\Omega}{2}t\right)\langle +z|-n\rangle \\ &= \cos^2\left(\frac{\theta}{2}\right)\exp\left(i\frac{\Omega}{2}t\right) + \sin^2\left(\frac{\theta}{2}\right)\exp\left(-i\frac{\Omega}{2}t\right) \\ &= \cos\left(\frac{\Omega}{2}t\right) + i\cos\theta\sin\left(\frac{\Omega}{2}t\right) \\ &= i\cos\theta\sin\left(\frac{t}{2}\sqrt{(\Delta\omega)^2 + \omega_1^2}\right) \end{aligned}$$

Then we have

$$\begin{aligned}
|\psi'(t)\rangle &= |+\rangle\langle+z|\psi'(t)\rangle + |-\rangle\langle-z|\psi'(t)\rangle \\
&= [\cos(\frac{\Omega}{2}t) + i \cos\theta \sin(\frac{\Omega}{2}t)]|+\rangle + i \sin\theta \sin(\frac{\Omega}{2}t)|-\rangle,
\end{aligned}$$

and

$$\begin{aligned}
|\psi(t)\rangle &= \hat{U}^+ |\psi'(t)\rangle \\
&= \begin{pmatrix} e^{\frac{i}{2}\omega t} & 0 \\ 0 & e^{-\frac{i}{2}\omega t} \end{pmatrix} \begin{pmatrix} \cos(\frac{\Omega}{2}t) + i \cos\theta \sin(\frac{\Omega}{2}t) \\ i \sin\theta \sin(\frac{\Omega}{2}t) \end{pmatrix} \\
&= \begin{pmatrix} e^{\frac{i}{2}\omega t} [\cos(\frac{\Omega}{2}t) + i \cos\theta \sin(\frac{\Omega}{2}t)] \\ e^{-\frac{i}{2}\omega t} i \sin\theta \sin(\frac{\Omega}{2}t) \end{pmatrix}
\end{aligned}$$

The Rabi's formula:

$P_-(t)$ is the probability for finding the spin in the state $|-\rangle$.

$P_+(t)$ is the probability for finding the spin in the state $|+\rangle$.

$$\begin{aligned}
P_-(t) &= |\langle -z | \psi(t) \rangle|^2 = |\langle -z | \psi'(t) \rangle|^2 \\
&= \sin^2 \theta \sin^2(\frac{\Omega t}{2}) \\
&= \sin^2 \theta \sin^2(\frac{t}{2} \sqrt{(\Delta\omega)^2 + \omega_1^2}) \\
&= \frac{\omega_1^2}{(\Delta\omega)^2 + \omega_1^2} \sin^2(\frac{t}{2} \sqrt{(\Delta\omega)^2 + \omega_1^2})
\end{aligned}$$

$$P_+(t) = |\langle +z | \psi(t) \rangle|^2 = |\langle +z | \psi'(t) \rangle|^2 = \cos^2(\frac{\Omega}{2}t) + \cos^2\theta \sin^2(\frac{\Omega}{2}t),$$

with

$$P_+(t) + P_-(t) = 1.$$

((Note))

$$\hat{U}(t)|+z\rangle = e^{-\frac{i}{2}\alpha t}|+z\rangle, \quad \hat{U}^+(t)|+z\rangle = e^{\frac{i}{2}\alpha t}|+z\rangle,$$

$$\hat{U}(t)|-z\rangle = e^{\frac{i}{2}\alpha t}|-z\rangle, \quad \hat{U}^+(t)|-z\rangle = e^{-\frac{i}{2}\alpha t}|-z\rangle.$$

Then we have

$$\langle +z|\psi'\rangle = \langle +z|\hat{U}|\psi\rangle = e^{-\frac{i}{2}\alpha t}\langle +z|\psi\rangle,$$

$$\langle -z|\psi'\rangle = \langle -z|\hat{U}|\psi\rangle = e^{\frac{i}{2}\alpha t}\langle -z|\psi\rangle,$$

or

$$|\langle +z|\psi'\rangle|^2 = \left| e^{-\frac{i}{2}\alpha t}\langle +z|\psi\rangle \right|^2 = |\langle +z|\psi\rangle|^2,$$

$$|\langle -z|\psi'\rangle|^2 = \left| e^{\frac{i}{2}\alpha t}\langle -z|\psi\rangle \right|^2 = |\langle -z|\psi\rangle|^2.$$

6. Derivation of the Rabi formula using the Mathematica

We calculate $\exp(-\frac{i\hat{H}'t}{\hbar})|\psi'(t=0)\rangle$, by using the Mathematica. This method is much simpler than the above method.

((Mathematica))

```
Clear["Global`*"]; exp_* := exp /. {Complex[re_, im_] :-> Complex[re, -im]};
H1 = \frac{\hbar}{2} \begin{pmatrix} \Delta\omega & -\omega_1 \\ -\omega_1 & -\Delta\omega \end{pmatrix}; M1 = MatrixExp[-\frac{i}{\hbar} H1 t] // FullSimplify;
rule1 = { \sqrt{-\Delta\omega^2 - \omega_1^2} -> i \Omega, \frac{1}{\sqrt{-\Delta\omega^2 - \omega_1^2}} -> \frac{-i}{\Omega} };
M2 = M1 /. rule1 // Simplify
{ {Cos[\frac{t \Omega}{2}] - \frac{i \Delta\omega Sin[\frac{t \Omega}{2}]}{\Omega}, \frac{i \omega_1 Sin[\frac{t \Omega}{2}]}{\Omega} }, { \frac{i \omega_1 Sin[\frac{t \Omega}{2}]}{\Omega}, Cos[\frac{t \Omega}{2}] + \frac{i \Delta\omega Sin[\frac{t \Omega}{2}]}{\Omega} } }
```

P11: Probability of finding in the state $|+z\rangle$

P21: Probability of finding in the state $|-z\rangle$

with

$$\sqrt{\Delta\omega^2 + \omega_1^2} = \Omega$$

$P1 = \{1, 0\} \cdot M2 \cdot \{1, 0\}$ // Simplify; $P11 = P1 * P1$ // Simplify

$$\cos\left[\frac{t\Omega}{2}\right]^2 + \frac{\Delta\omega^2 \sin\left[\frac{t\Omega}{2}\right]^2}{\Omega^2}$$

$P2 = \{0, 1\} \cdot M2 \cdot \{1, 0\}$ // Simplify; $P21 = P2 * P2$ // Simplify

$$\frac{\omega_1^2 \sin\left[\frac{t\Omega}{2}\right]^2}{\Omega^2}$$

6. Summary

We use the Mathematica (see the **Appendix**) to solve the above problem. The results are as follows.

$$\Omega = \sqrt{(\Delta\omega)^2 + \omega_1^2},$$

$$\Delta\omega = \omega_0 - \omega,$$

$$|\psi'(t)\rangle = \begin{pmatrix} b_1(t) \\ b_2(t) \end{pmatrix} = \exp\left(-\frac{i\hat{H}'t}{\hbar}\right)|\psi(t=0)\rangle,$$

where

$$\exp\left(-\frac{i\hat{H}'t}{\hbar}\right) = \begin{pmatrix} \frac{\Omega \cos\left(\frac{\Omega}{2}t\right) - i\Delta\omega \sin\left(\frac{\Omega}{2}t\right)}{\Omega} & i\frac{\omega_1}{\Omega} \sin\left(\frac{\Omega}{2}t\right) \\ i\frac{\omega_1}{\Omega} \sin\left(\frac{\Omega}{2}t\right) & \frac{\Omega \cos\left(\frac{\Omega}{2}t\right) + i\Delta\omega \sin\left(\frac{\Omega}{2}t\right)}{\Omega} \end{pmatrix}.$$

We assume that

$$|\psi(t=0)\rangle = |+\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

$$|\psi'(t)\rangle = \begin{pmatrix} b_1(t) \\ b_2(t) \end{pmatrix} = \exp\left(-\frac{i\hat{H}'t}{\hbar}\right) \begin{pmatrix} 1 \\ 0 \end{pmatrix},$$

$$P_- = |b_2|^2 = \frac{\omega_1^2 \sin^2\left(\frac{\Omega}{2}t\right)}{\Omega^2}.$$

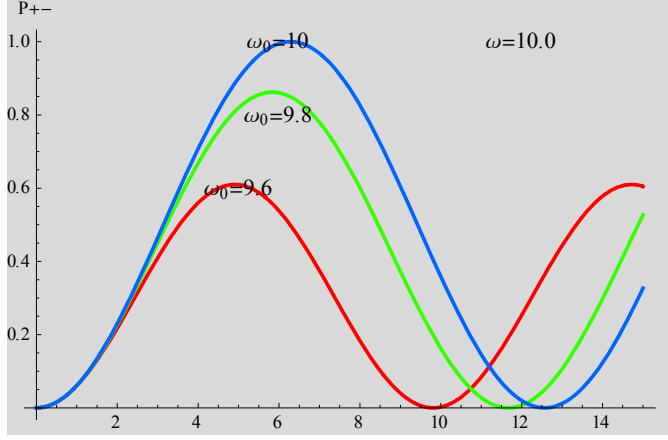


Fig. $P_- = P_-$ vs t . $\omega_1 = 0.5$. $\omega = 10$. ω_0 is changed as a parameter.

$$P_- = |b_1|^2 = 1 - \frac{\omega_1^2 \sin^2\left(\frac{\Omega}{2}t\right)}{\Omega^2}.$$

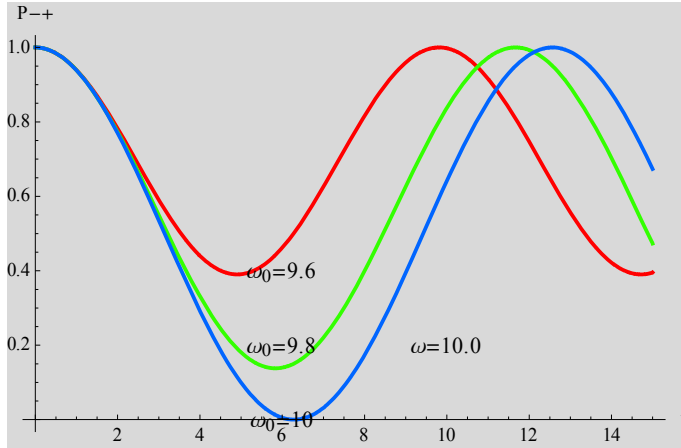


Fig. $P_+ vs t$. $\omega_1 = 0.5$. $\omega = 10$. ω_0 is changed as a parameter.

The state vector is given by

$$|\psi(t)\rangle = \hat{U}^+ \exp\left(-\frac{i\hat{H}'t}{\hbar}\right)|\psi(t=0)\rangle$$

$$= \begin{pmatrix} \frac{e^{\frac{1}{2}i(\omega-\Omega)t}}{2\Omega} [\Omega + \Delta\omega + e^{i\Omega t}(\Omega - \Delta\omega)] \\ i \frac{\omega_1}{\Omega} e^{-\frac{1}{2}i\omega t} \sin\left(\frac{\Omega t}{2}\right) \end{pmatrix}.$$

7. Expectation values

The expectation value

$$\begin{aligned}\langle I_z \rangle &= \frac{1}{2} \langle \psi(t) | \hat{\sigma}_z | \psi(t) \rangle \\ &= \frac{1}{4\Omega^2} [(\Delta\omega)^2 + \Omega^2 - \omega_1^2 + (-\Delta\omega)^2 + \Omega^2 + \omega_1^2] \cos(\Omega t)\end{aligned}$$

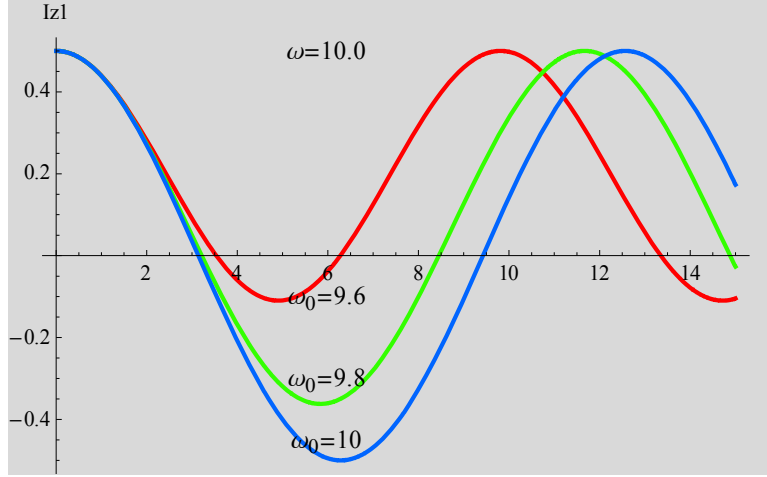


Fig. $\langle I_z \rangle$ vs t . $\omega_1 = 0.5$. $\omega = 10$. ω_0 is changed as a parameter.

$$\begin{aligned}\langle I_x \rangle &= \frac{1}{2} \langle \psi(t) | \hat{\sigma}_x | \psi(t) \rangle \\ &= \frac{\omega_1}{\Omega^2} [-\Delta\omega \cos(\omega t) \sin^2\left(\frac{\Omega t}{2}\right) + \frac{1}{2} \Omega \sin(\omega t) \sin(\Omega t)]\end{aligned}$$

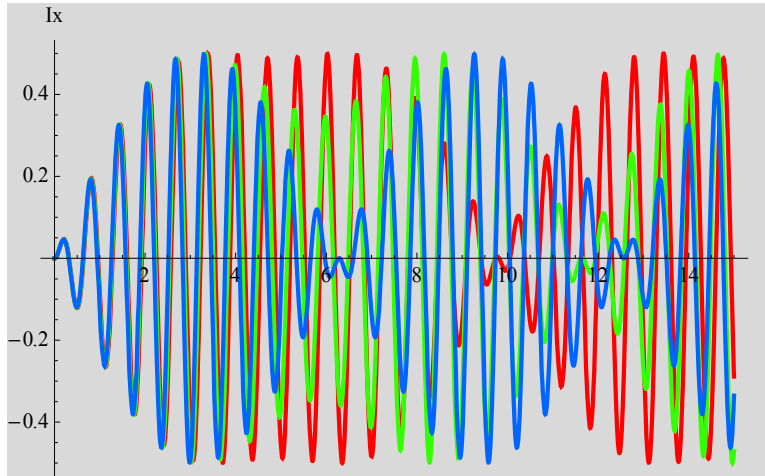


Fig. $\langle I_x \rangle$ vs t . $\omega_1 = 0.5$. $\omega = 10$. ω_0 is changed as a parameter.

$$\langle I_y \rangle = \frac{1}{2} \langle \psi(t) | \hat{\sigma}_y | \psi(t) \rangle = \frac{\omega_1}{\Omega^2} [\Delta \omega \sin(\omega t) \sin^2\left(\frac{\Omega t}{2}\right) + \frac{1}{2} \Omega \omega_1 \cos(\omega t) \sin(\Omega t)].$$

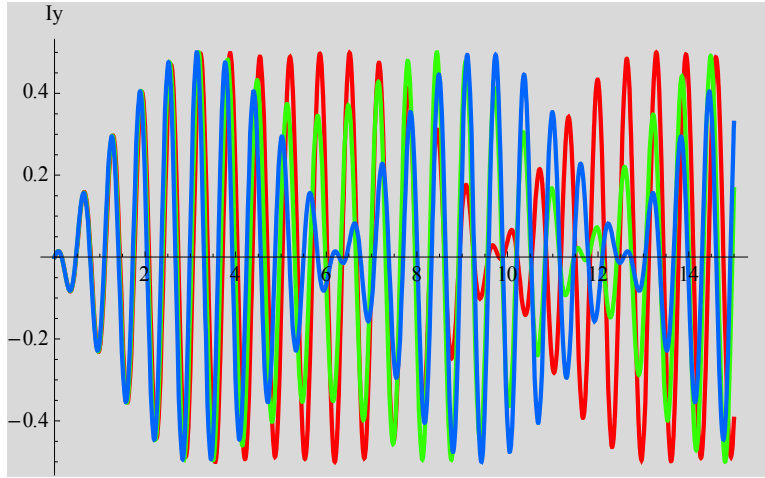


Fig. $\langle I_y \rangle$ vs t . $\omega_1 = 0.5$. $\omega = 10$. ω_0 is changed as a parameter.

8. The notation used by Townsend (in the textbook)

In Townsend book, the magnetic field is given by

$$\mathbf{B}_1' = B_1' \cos(\omega t) \mathbf{e}_x, \quad (\text{linearly polarized}),$$

leading to

$$\omega_1' = \gamma B_1'.$$

In the present case we assume that

$$\mathbf{B}_1 = 2 B_1 \cos(\omega t) \mathbf{e}_x, \quad (\text{linearly polarized})$$

leading to

$$\omega_1 = \gamma B_1.$$

Since

$$B_1' = 2B_1,$$

the relation between ω_1' and ω_1 is given by

$$\frac{\omega_1}{\omega_1'} = \frac{B_1}{B_1'} = \frac{1}{2}.$$

Therefore the Rabi frequency can be expressed by

$$\Omega = \sqrt{(\Delta\omega)^2 + \frac{\omega_1'^2}{4}},$$

where

$$\Delta\omega = \omega - \omega_0.$$

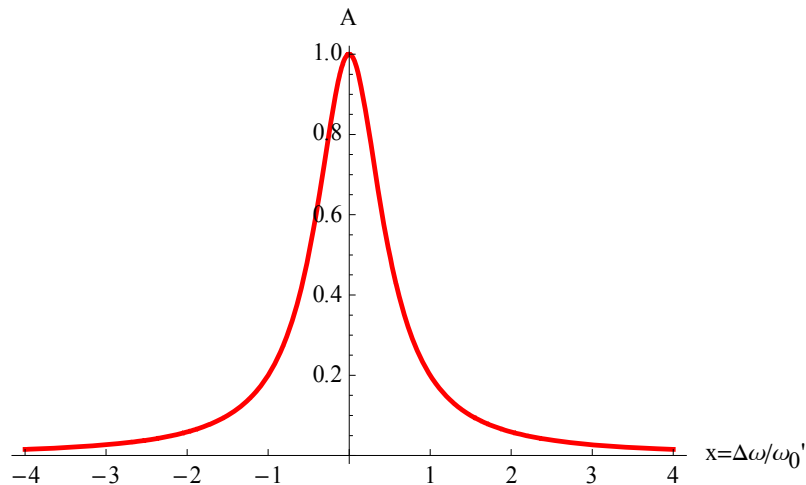
The probability is

$$P_{+\rightarrow-}(t) = \frac{\omega_1'^2/4}{(\Delta\omega)^2 + \omega_1'^2/4} \sin^2\left(\frac{t}{2}\sqrt{(\Delta\omega)^2 + \omega_1'^2/4}\right).$$

(Rabi's formula in Townsend book). The amplitude of $P_{+\rightarrow-}(t)$ is equal to

$$A = \frac{\frac{1}{4}}{\frac{(\Delta\omega)^2}{\omega_1'^2} + \frac{1}{4}}.$$

We make a plot of A as a function of $x = \Delta\omega/\omega_1'$.



9. Example-1 ((Mathematica))

All the procedures described above, can be done directly by using the Mathematica. We can get the results shown in Section 7 described above.

((Mathematica))

```

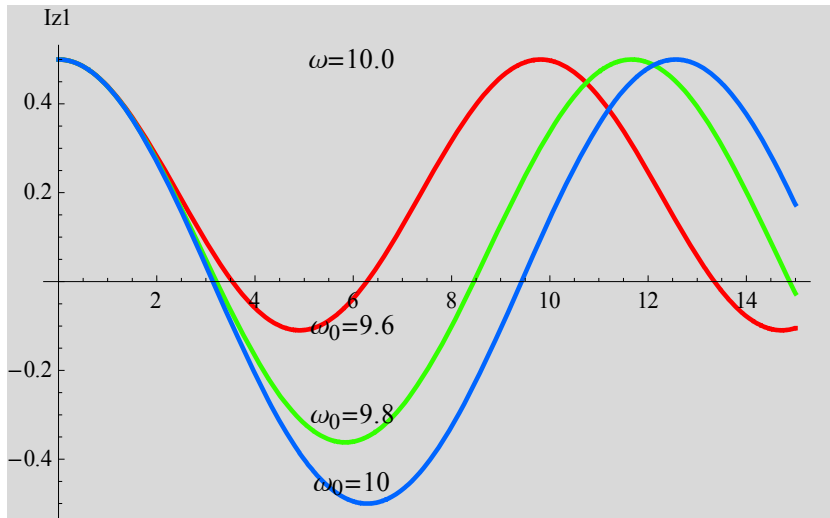
Clear["Global`*"]; SuperStar;
expr_* := expr /. Complex[a_, b_] :=> Complex[a, -b]; Xa = {a1[t], a2[t]};
H1 =  $\frac{\hbar}{2}$  {{ $\Delta\omega$ ,  $-\omega_1$ }, {- $\omega_1$ ,  $-\Delta\omega$ }};  $\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$ ;  $\sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$ ;
 $\sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$ ; rule1 = { $\sqrt{-\Delta\omega^2 - \omega_1^2} \rightarrow i \Omega$ ,  $\frac{1}{\sqrt{-\Delta\omega^2 - \omega_1^2}} \rightarrow -i \frac{1}{\Omega}$ };
rule2 = { $\Omega \rightarrow \sqrt{\Delta\omega^2 + \omega_1^2}$ ,  $\Delta\omega \rightarrow (\omega - \omega_0)$ ,  $\omega_1 \rightarrow 0.5$ ,  $\omega \rightarrow 10$ };
A1 = MatrixExp[ $\frac{i}{2} \omega t \sigma_z$ ].MatrixExp[ $-\frac{i}{\hbar} H1 t$ ] /. rule1 // FullSimplify;
 $\psi_1 = A1.\{1, 0\}$  // ComplexExpand // FullSimplify
{ $\frac{e^{\frac{i t \omega}{2}} (\Omega \cos[\frac{t \Omega}{2}] - i \Delta\omega \sin[\frac{t \Omega}{2}])}{\Omega}$ ,  $\frac{i e^{-\frac{1}{2} i t \omega} \omega_1 \sin[\frac{t \Omega}{2}]}{\Omega}$ }
Ix =  $\frac{1}{2} \psi_1^* .\sigma_x.\psi_1$  // ComplexExpand // FullSimplify
 $\frac{\omega_1 (-2 \Delta\omega \cos[t \omega] \sin[\frac{t \Omega}{2}]^2 + \Omega \sin[t \omega] \sin[t \Omega])}{2 \Omega^2}$ 
Iy =  $\frac{1}{2} \psi_1^* .\sigma_y.\psi_1$  // FullSimplify
 $\frac{\Delta\omega \omega_1 \sin[t \omega] \sin[\frac{t \Omega}{2}]^2 + \frac{1}{2} \Omega \omega_1 \cos[t \omega] \sin[t \Omega]}{\Omega^2}$ 
Iz =  $\frac{1}{2} \psi_1^* .\sigma_z.\psi_1$  // ComplexExpand // FullSimplify
 $\frac{1}{2} \left( \cos[\frac{t \Omega}{2}]^2 + \frac{(\Delta\omega - \omega_1) (\Delta\omega + \omega_1) \sin[\frac{t \Omega}{2}]^2}{\Omega^2} \right)$ 

```

```

Iz1 = Iz //. rule2;
k1 = Plot[Evaluate[Table[Iz1, { $\omega_0$ , 9.6, 10, 0.2}]], {t, 0, 15},
  PlotStyle -> Table[{Thick, Hue[0.3 i]}, {i, 0, 20}],
  Background -> LightGray, AxesLabel -> {"t", "Iz1"}, PlotRange -> All];
k2 = Graphics[{Text[Style[" $\omega_0=10$ ", Black, 12], {6, -0.45}],
  Text[Style[" $\omega_0=9.8$ ", Black, 12], {6, -0.30}],
  Text[Style[" $\omega_0=9.6$ ", Black, 12], {6, -0.1}],
  Text[Style[" $\omega=10.0$ ", Black, 12], {6, 0.5}]];
Show[k1, k2]

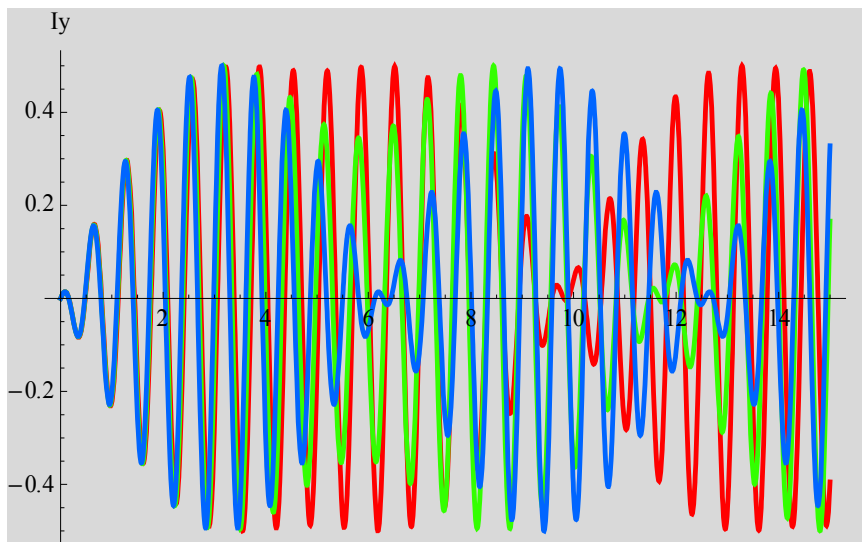
```



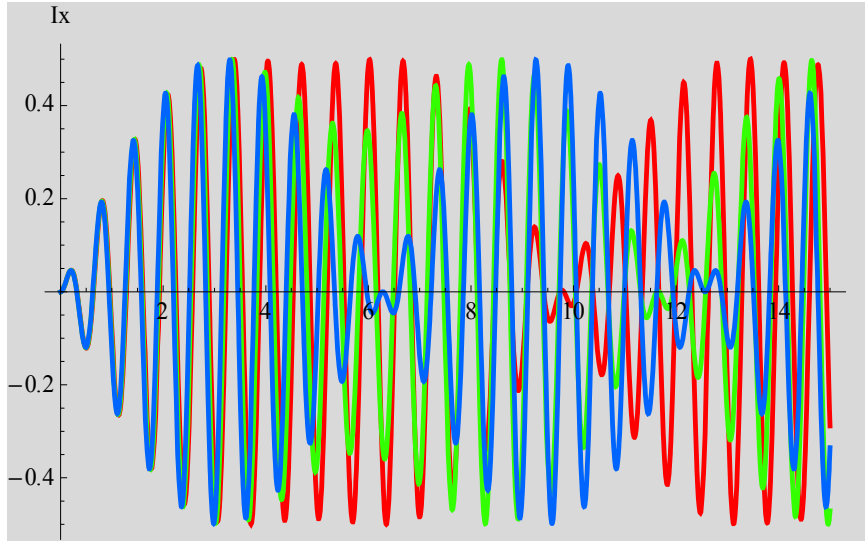
```

Iy1 = Iy //. rule2;
p1 = Plot[Evaluate[Table[Iy1, { $\omega_0$ , 9.6, 10, 0.2}]], {t, 0, 15},
  PlotStyle -> Table[{Thick, Hue[0.3 i]}, {i, 0, 20}],
  Background -> LightGray, AxesLabel -> {"t", "Iy"}, PlotRange -> All]

```



```
Ix1 = Ix //. rule2;  
p2 = Plot[Evaluate[Table[Ix1, {ω0, 9.6, 10, 0.2}]], {t, 0, 15},  
PlotStyle → Table[{Thick, Hue[0.3 i]}, {i, 0, 20}],  
Background → LightGray, AxesLabel → {"t", "Ix"}, PlotRange → All]
```

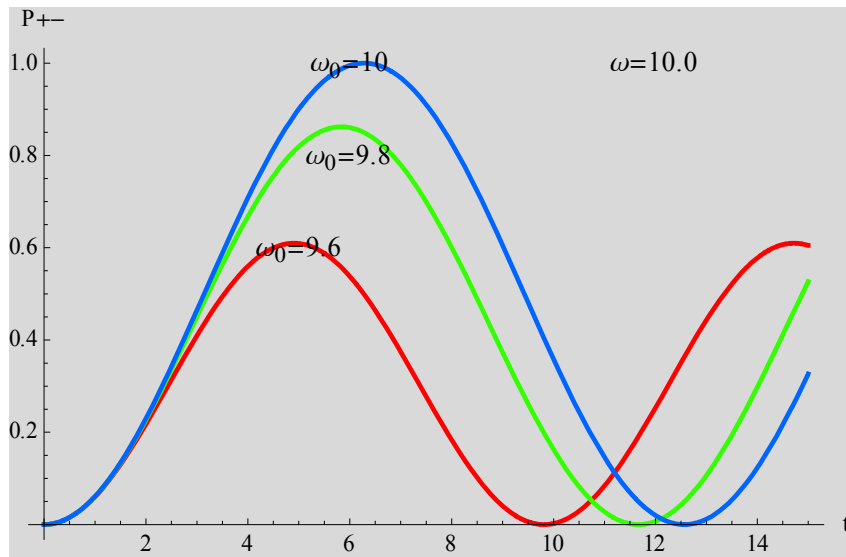



```

B1 = MatrixExp[- $\frac{i}{\hbar}$  H1 t] /. rule1 // FullSimplify; P1 = {0, 1}.B1.{1, 0};
P11 = Abs[P1]2;
P12 = P11 /. rule2;

h1 = Plot[Evaluate[Table[P12, { $\omega_0$ , 9.6, 10, 0.2}]], {t, 0, 15},
  PlotStyle -> Table[{Thick, Hue[0.3 i]}, {i, 0, 20}],
  Background -> LightGray, AxesLabel -> {"t", "P+-"}, PlotRange -> All];
h2 = Graphics[{Text[Style[" $\omega_0=10$ ", Black, 12], {6, 1}],
  Text[Style[" $\omega_0=9.8$ ", Black, 12], {6, 0.8}],
  Text[Style[" $\omega_0=9.6$ ", Black, 12], {5, 0.6}],
  Text[Style[" $\omega=10.0$ ", Black, 12], {12, 1}]}];
Show[h1, h2]

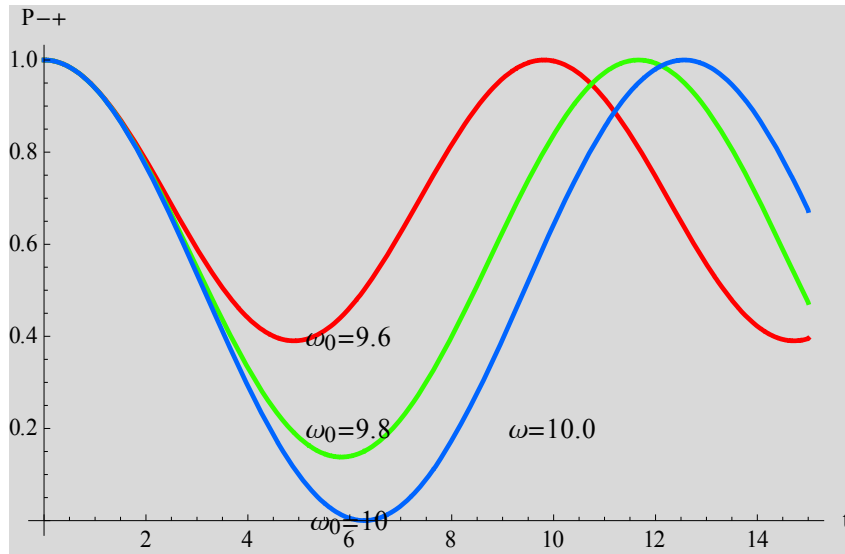
```



```

h3 = Plot[Evaluate[Table[1 - P12, { $\omega_0$ , 9.6, 10, 0.2}]], {t, 0, 15},
  PlotStyle -> Table[{Thick, Hue[0.3 i]}, {i, 0, 20}],
  Background -> LightGray, AxesLabel -> {"t", "P-+"}, PlotRange -> All];
h4 = Graphics[{Text[Style[" $\omega_0=10$ ", Black, 12], {6, 0}],
  Text[Style[" $\omega_0=9.8$ ", Black, 12], {6, 0.2}],
  Text[Style[" $\omega_0=9.6$ ", Black, 12], {6, 0.4}],
  Text[Style[" $\omega=10.0$ ", Black, 12], {10, 0.2}]}];
Show[h3, h4]

```



10. Example-2 ((Mathematica))

All the procedures described above, can be done directly by using another Mathematica program.

eq3 = eq1 - eq2 // Simplify

$$\left\{ \frac{1}{2} e^{\frac{i t \omega}{2}} (i (\omega - \omega_0) b_1[t] - i \omega_1 b_2[t] + 2 b_1'[t]), \right. \\ \left. - \frac{1}{2} i e^{-\frac{1}{2} i t \omega} (\omega_1 b_1[t] + (\omega - \omega_0) b_2[t] + 2 i b_2'[t]) \right\}$$

Solve[eq3[[1]] == 0, b1'[t]] // Simplify

$$\left\{ \left\{ b_1'[t] \rightarrow \frac{1}{2} i ((-\omega + \omega_0) b_1[t] + \omega_1 b_2[t]) \right\} \right\}$$

Solve[eq3[[2]] == 0, b2'[t]] // Simplify

$$\left\{ \left\{ b_2'[t] \rightarrow \frac{1}{2} i (\omega_1 b_1[t] + (\omega - \omega_0) b_2[t]) \right\} \right\}$$

New matrix

$$\mathbf{NM} = \left\{ \left\{ \frac{1}{2} i (\omega_0 - \omega), \frac{1}{2} i \omega_1 \right\}, \left\{ \frac{1}{2} i \omega_1, \frac{1}{2} i (\omega - \omega_0) \right\} \right\};$$

We have now the equation of motion for the new state vector

$$\mathbf{rule2} = \left\{ \sqrt{-\omega^2 + 2 \omega \omega_0 - \omega_0^2 - \omega_1^2} \rightarrow i \Omega, \frac{1}{\sqrt{-\omega^2 + 2 \omega \omega_0 - \omega_0^2 - \omega_1^2}} \rightarrow -i \frac{1}{\Omega} \right\};$$

EE = MatrixExp[NM t] /. rule2 // ExpToTrig // Simplify

$$\left\{ \left\{ \frac{\Omega \operatorname{Cos}\left[\frac{t\Omega}{2}\right] - i(\omega - \omega_0) \operatorname{Sin}\left[\frac{t\Omega}{2}\right]}{\Omega}, \frac{i\omega_1 \operatorname{Sin}\left[\frac{t\Omega}{2}\right]}{\Omega} \right\}, \left\{ \frac{i\omega_1 \operatorname{Sin}\left[\frac{t\Omega}{2}\right]}{\Omega}, \frac{\Omega \operatorname{Cos}\left[\frac{t\Omega}{2}\right] + i(\omega - \omega_0) \operatorname{Sin}\left[\frac{t\Omega}{2}\right]}{\Omega} \right\} \right\}$$

ψ1 = EE.{1, 0} // Simplify

$$\left\{ \frac{\Omega \operatorname{Cos}\left[\frac{t\Omega}{2}\right] - i(\omega - \omega_0) \operatorname{Sin}\left[\frac{t\Omega}{2}\right]}{\Omega}, \frac{i\omega_1 \operatorname{Sin}\left[\frac{t\Omega}{2}\right]}{\Omega} \right\}$$

C1 = ψ1[[1]]

$$\frac{\Omega \operatorname{Cos}\left[\frac{t\Omega}{2}\right] - i(\omega - \omega_0) \operatorname{Sin}\left[\frac{t\Omega}{2}\right]}{\Omega}$$

C2 = ψ1[[2]]

$$\frac{i\omega_1 \operatorname{Sin}\left[\frac{t\Omega}{2}\right]}{\Omega}$$

rule3 = {ω² - 2 ω ω₀ + ω₀² → Ω² - ω₁²};

P1 = C1* C1 // ExpToTrig // Simplify /. rule3

$$\frac{\omega^2 + \Omega^2 - 2\omega\omega_0 + \omega_0^2 - (\omega^2 - \Omega^2 - 2\omega\omega_0 + \omega_0^2) \operatorname{Cos}[t\Omega]}{2\Omega^2}$$

```
P2 = C2* C2 // ExpToTrig // Simplify
```

$$\frac{\omega_1^2 \sin\left[\frac{t\Omega}{2}\right]^2}{\Omega^2}$$

```
P1 + P2 //. rule3 // Simplify
```

```
1
```

The final result is as follows.

$$P2 = \frac{\omega_1^2 \sin\left[\frac{t\Omega}{2}\right]^2}{\Omega^2} \text{ and } P1 = 1 - P2 *$$

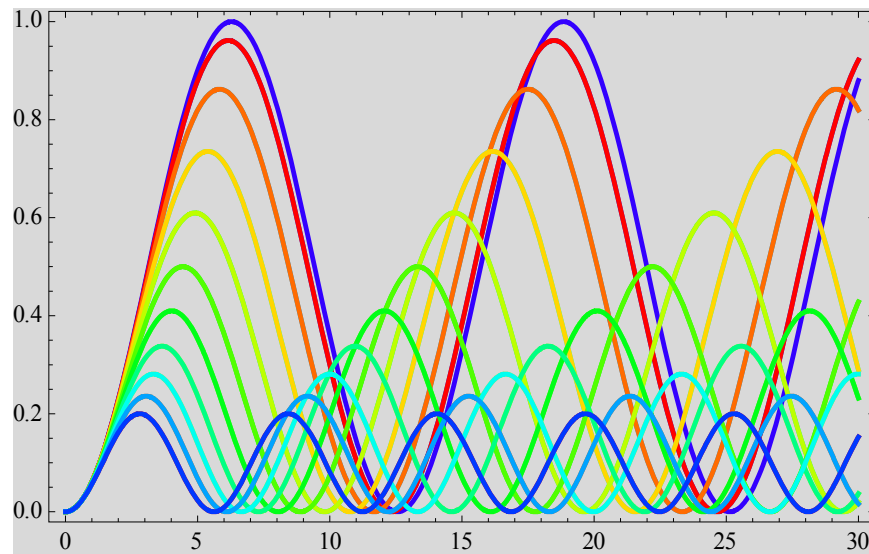
```
rule5 = {Ω → √{ω² - 2 ω ω0 + ω0² + ω1²}};
```

```
P21 = P2 /. rule5;
```

```
rule6 = {ω1 → 0.5, ω → 10};
```

```
P22 = P21 /. rule6;
```

```
Plot[Evaluate[Table[P22, {ω0, 9, 11, 0.1}]], {t, 0, 30},
PlotStyle → Table[{Thick, Hue[0.07 i]}, {i, 0, 10}],
Background → LightGray, Frame → True]
```



11. Nuclear magnetic resonance based on the Dirac picture

11.1 Solving the problem in the Dirac picture

The Hamiltonian is given by

$$\hat{H} = \hat{H}_0 + \hat{V}(t),$$

where \hat{H}_0 is independent of t . The wavefunctions in the Schrödinger picture and in the Dirac picture are related by

$$|\psi_s(t)\rangle = e^{-\frac{i}{\hbar}\hat{H}_0 t} |\psi_I(t)\rangle,$$

or

$$|\psi_I(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t} |\psi_s(t)\rangle.$$

The Schrödinger equation is given by

$$i\hbar \frac{\partial}{\partial t} |\psi_I(t)\rangle = i\hbar \frac{\partial}{\partial t} e^{\frac{i}{\hbar}\hat{H}_0 t} |\psi_s(t)\rangle = -\hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t} |\psi_s(t)\rangle + e^{\frac{i}{\hbar}\hat{H}_0 t} i\hbar \frac{\partial}{\partial t} |\psi_s(t)\rangle.$$

Since

$$i\hbar \frac{\partial}{\partial t} |\psi_s(t)\rangle = [\hat{H}_0 + \hat{V}(t)] |\psi_s(t)\rangle$$

then we get

$$i\hbar \frac{\partial}{\partial t} |\psi_I(t)\rangle = -\hat{H}_0 e^{\frac{i}{\hbar}\hat{H}_0 t} |\psi_s(t)\rangle + e^{\frac{i}{\hbar}\hat{H}_0 t} [\hat{H}_0 + \hat{V}(t)] |\psi_s(t)\rangle,$$

or

$$i\hbar \frac{\partial}{\partial t} |\psi_I(t)\rangle = e^{\frac{i}{\hbar}\hat{H}_0 t} \hat{V}(t) e^{-\frac{i}{\hbar}\hat{H}_0 t} |\psi_I(t)\rangle = \hat{V}_I(t) |\psi_I(t)\rangle,$$

or

$$i\hbar \frac{\partial}{\partial t} |\psi_I(t)\rangle = \hat{V}_I(t) |\psi_I(t)\rangle,$$

where

$$\hat{V}_I(t) = e^{\frac{i}{\hbar}\hat{H}_0 t} \hat{V}(t) e^{-\frac{i}{\hbar}\hat{H}_0 t} \quad (\text{Heisenberg-like})$$

11.2 The form of $\hat{V}_I(t)$

The Hamiltonian \hat{H} is given by

$$\begin{aligned} \hat{H} &= -\boldsymbol{\mu} \cdot \mathbf{B}(t) \\ &= -\gamma \frac{\hbar}{2} (\mathbf{B} \cdot \hat{\boldsymbol{\sigma}}) \\ &= -\gamma \frac{\hbar}{2} [B_0 \hat{\sigma}_z + B_1 \cos(\omega t) \hat{\sigma}_x - B_1 \sin(\omega t) \hat{\sigma}_y] \end{aligned}$$

or

$$\hat{H} = -\frac{\hbar}{2} \begin{pmatrix} \gamma B_0 & \gamma B_1 e^{i\omega t} \\ \gamma B_1 e^{-i\omega t} & -\gamma B_0 \end{pmatrix} = -\frac{\hbar}{2} \begin{pmatrix} \omega_0 & \omega_1 e^{i\omega t} \\ \omega_1 e^{-i\omega t} & -\omega_0 \end{pmatrix},$$

where

$$\omega_0 = \gamma B_0, \quad \omega_1 = \gamma B_1.$$

Then the Hamiltonian is rewritten as

$$\hat{H} = -\frac{\hbar}{2} \omega_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} - \frac{\hbar}{2} \omega_1 \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix} = \hat{H}_0 + \hat{V},$$

where

$$\hat{H}_0 = -\frac{\hbar}{2} \omega_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} = -\frac{\hbar}{2} \omega_0 \hat{\sigma}_z, \quad \hat{V} = -\frac{\hbar}{2} \omega_1 \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix}.$$

Under the basis of $\{|+z\rangle$ and $\{|-z\rangle$, we have

$$\hat{H}_0 | +z \rangle = -\frac{1}{2} \hbar \omega_0 | +z \rangle, \quad \hat{H}_0 | -z \rangle = \frac{1}{2} \hbar \omega_0 | -z \rangle,$$

and

$$\begin{aligned}
\hat{V}_I(t) &= e^{\frac{i}{\hbar}\hat{H}_0 t} \hat{V}(t) e^{-\frac{i}{\hbar}\hat{H}_0 t} \\
&= -\frac{1}{2}\hbar\omega_1 \begin{pmatrix} e^{-i\omega_0 t/2} & 0 \\ 0 & e^{i\omega_0 t/2} \end{pmatrix} \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix} \begin{pmatrix} e^{i\omega_0 t/2} & 0 \\ 0 & e^{-i\omega_0 t/2} \end{pmatrix} \\
&= -\frac{1}{2}\hbar\omega_1 \begin{pmatrix} 0 & e^{i(\omega-\omega_0)t} \\ e^{-i(\omega-\omega_0)t} & 0 \end{pmatrix}
\end{aligned}$$

11.3 The wave functions $|\psi_S(t)\rangle$ and $|\psi_I(t)\rangle$

We assume the wave function:

$$|\psi_S(t)\rangle = \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} = a_1(t)|+z\rangle + a_2(t)|-z\rangle,$$

$$\begin{aligned}
|\psi_I(t)\rangle &= e^{\frac{i}{\hbar}\hat{H}_0 t} |\psi_S(t)\rangle \\
&= e^{\frac{i}{\hbar}\hat{H}_0 t} [a_1(t)|+z\rangle + a_2(t)|-z\rangle] \\
&= e^{-\frac{i}{2}\omega_0 t} a_1(t)|+z\rangle + e^{\frac{i}{2}\omega_0 t} a_2(t)|-z\rangle \\
&= b_1(t)|+z\rangle + b_2(t)|-z\rangle
\end{aligned}$$

where

$$e^{-\frac{i}{2}\omega_0 t} a_1(t) = b_1(t), \quad e^{\frac{i}{2}\omega_0 t} a_2(t) = b_2(t),$$

or

$$a_1(t) = e^{\frac{i}{2}\omega_0 t} b_1(t), \quad a_2(t) = e^{-\frac{i}{2}\omega_0 t} b_2(t).$$

We now solve the differential equation

$$i\hbar \frac{\partial}{\partial t} |\psi_I(t)\rangle = \hat{V}_I(t) |\psi_I(t)\rangle,$$

or

$$i\hbar \begin{pmatrix} \dot{b}_1(t) \\ \dot{b}_2(t) \end{pmatrix} = -\frac{1}{2}\hbar\omega_1 \begin{pmatrix} 0 & e^{i(\omega-\omega_0)t} \\ e^{-i(\omega-\omega_0)t} & 0 \end{pmatrix} \begin{pmatrix} b_1(t) \\ b_2(t) \end{pmatrix},$$

or

$$\begin{pmatrix} \dot{b}_1(t) \\ \dot{b}_2(t) \end{pmatrix} = \frac{1}{2}i\omega_1 \begin{pmatrix} 0 & e^{i(\omega-\omega_0)t} \\ e^{-i(\omega-\omega_0)t} & 0 \end{pmatrix} \begin{pmatrix} b_1(t) \\ b_2(t) \end{pmatrix} = \frac{1}{2}i\omega_1 \begin{pmatrix} e^{i(\omega-\omega_0)t}b_2(t) \\ e^{-i(\omega-\omega_0)t}b_1(t) \end{pmatrix}.$$

We solve this differential equations by using the Mathematica.

$$\Delta = \omega - \omega_0, \quad \Omega = \sqrt{\omega_1^2 + \Delta^2}.$$

We assume the initial condition; $b_1(0) = 1$, $b_2(0) = 0$

$$b_1(t) = \frac{1}{\Omega} e^{i\Delta t/2} [\Omega \cos(\frac{\Omega t}{2}) - i\Delta \sin(\frac{\Omega t}{2})],$$

$$b_2(t) = \frac{i\omega_1}{\Omega} e^{i\Delta t/2} \sin(\frac{\Omega t}{2}).$$

The probability:

$$P_1(t) = |b_1(t)|^2 = 1 - \frac{\omega_1^2}{\Omega^2} \sin^2(\frac{\Omega t}{2}),$$

$$P_2(t) = |b_2(t)|^2 = \frac{\omega_1^2}{\Omega^2} \sin^2(\frac{\Omega t}{2}).$$

((Mathematica))

```

Clear["Global`*"]; SuperStar;
expr_* := expr /. Complex[a_, b_] := Complex[a, -b];

 $\Delta = \omega - \omega_0, \quad \sqrt{\omega_1^2 + \Delta^2} = \Omega,$ 

eq1 = D[b1[t], t] ==  $\frac{i}{2} \omega_1 \text{Exp}[i \Delta t] b_2[t];$ 
eq2 = D[b2[t], t] ==  $\frac{i}{2} \omega_1 \text{Exp}[-i \Delta t] b_1[t];$ 

s11 = DSolve[{eq1, eq2, b1[0] == 1, b2[0] == 0},
  {b1[t], b2[t]}, t // Simplify[#, { $\Delta > 0, \omega_1 > 0$ }] &;
s12 = s11 /. { $\sqrt{\omega_1^2 + \Delta^2} \rightarrow \Omega, \frac{1}{\sqrt{\omega_1^2 + \Delta^2}} \rightarrow \frac{1}{\Omega}$ } // Simplify;

b1[t_] = b1[t] /. s12[[1]] // ComplexExpand //
  FullSimplify

$$\frac{e^{\frac{i t \Delta}{2}} \left( \Omega \text{Cos}\left[\frac{t \Omega}{2}\right] - i \Delta \text{Sin}\left[\frac{t \Omega}{2}\right] \right)}{\Omega}$$


```

b2[t_] = b2[t] /. s12[[1]] // ComplexExpand // FullSimplify

$$\frac{i e^{-\frac{1}{2} i t \Delta} \omega_1 \operatorname{Sin}\left[\frac{t \Omega}{2}\right]}{\Omega}$$

P1 = b1[t] * b1[t] // ComplexExpand // FullSimplify

$$\operatorname{Cos}\left[\frac{t \Omega}{2}\right]^2 + \frac{\Delta^2 \operatorname{Sin}\left[\frac{t \Omega}{2}\right]^2}{\Omega^2}$$

P11 = P1 /. {Ω → √(ω1² + Δ²)} // Simplify

$$\frac{2 \Delta^2 + \omega_1^2 + \omega_1^2 \operatorname{Cos}\left[t \sqrt{\Delta^2 + \omega_1^2}\right]}{2 (\Delta^2 + \omega_1^2)}$$

P2 = b2[t] * b2[t] // TrigFactor

$$\frac{\omega_1^2 \operatorname{Sin}\left[\frac{t \Omega}{2}\right]^2}{\Omega^2}$$

```
P21 = P2 /. {Ω → √(ω12 + Δ2) } // Simplify
```

$$\frac{\omega_1^2 \sin\left[\frac{1}{2} t \sqrt{\Delta^2 + \omega_1^2}\right]^2}{\Delta^2 + \omega_1^2}$$

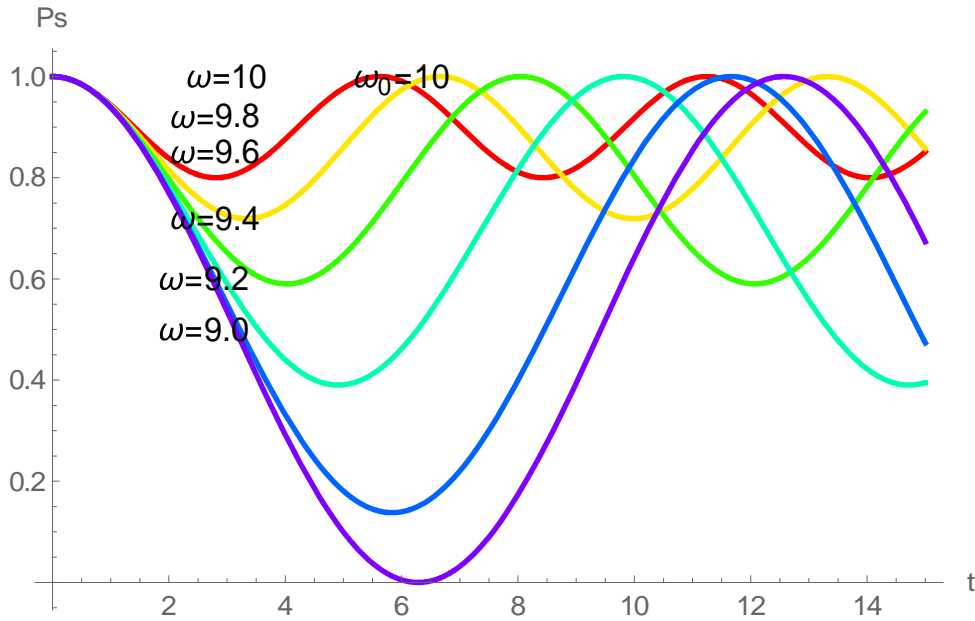
```
P11 + P21 // Simplify
```

```
1
```

```
ga11 = P11 /. {Δ → ω - ω0, ω0 → 10, ω1 → 0.5}
```

$$\frac{0.25 + 2(-10 + \omega)^2 + 0.25 \cos\left[t \sqrt{0.25 + (-10 + \omega)^2}\right]}{2(0.25 + (-10 + \omega)^2)}$$

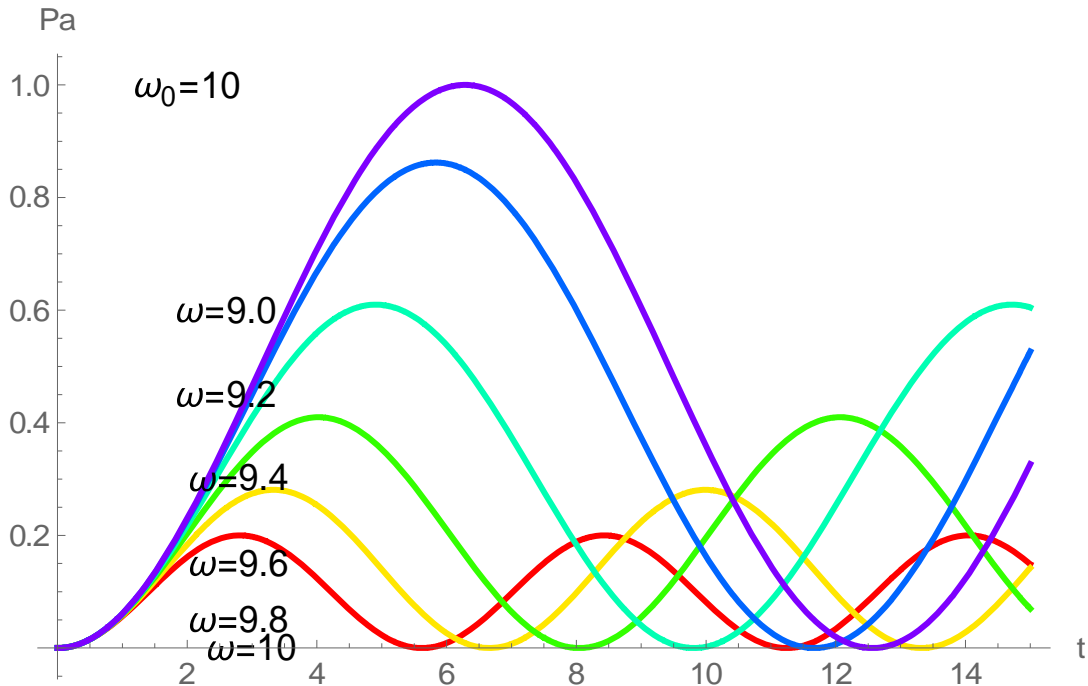
```
f1 = Plot[Evaluate[Table[ga11, {ω, 9, 10, 0.2}]],
  {t, 0, 15},
  PlotStyle → Table[{Thick, Hue[0.15 i]}, {i, 0, 5}],
  AxesLabel → {"t", "Ps"}];
f2 = Graphics[{Text[Style["ω0=10", Black, 12], {6, 1}],
  Text[Style["ω=10", Black, 12], {3, 1}],
  Text[Style["ω=9.8", Black, 12], {2.8, 0.92}],
  Text[Style["ω=9.6", Black, 12], {2.8, 0.85}],
  Text[Style["ω=9.4", Black, 12], {2.8, 0.72}],
  Text[Style["ω=9.2", Black, 12], {2.6, 0.6}],
  Text[Style["ω=9.0", Black, 12], {2.6, 0.5}]]];
Show[f1, f2]
```



```

f1 = Plot[Evaluate[Table[1 - ga11, { $\omega$ , 9, 10, 0.2}]],
  {t, 0, 15},
  PlotStyle -> Table[{Thick, Hue[0.15 i]}, {i, 0, 5}],
  AxesLabel -> {"t", "Pa"}];
f2 = Graphics[{Text[Style[" $\omega_0=10$ ", Black, 12], {2, 1}],
  Text[Style[" $\omega=10$ ", Black, 12], {3, 0}],
  Text[Style[" $\omega=9.8$ ", Black, 12], {2.8, 0.05}],
  Text[Style[" $\omega=9.6$ ", Black, 12], {2.8, 0.15}],
  Text[Style[" $\omega=9.4$ ", Black, 12], {2.8, 0.3}],
  Text[Style[" $\omega=9.2$ ", Black, 12], {2.6, 0.45}],
  Text[Style[" $\omega=9.0$ ", Black, 12], {2.6, 0.6}]];
Show[f1, f2]

```



REFERENCES

1. Claude Cohen-Tannoudji, Bernard Diu, and Franck Laloë, *Quantum Mechanics*, volume I and volume II (John Wiley & Sons, New York, 1977).
2. J.J. Sakurai and J. Napolitano, *Modern Quantum Mechanics*, second edition (Addison-Wesley, New York, 2011).
3. John S. Townsend, *A Modern Approach to Quantum Mechanics*, second edition (University Science Books, 2012).
4. David H. McIntyre, *Quantum Mechanics A Paradigms Approach* (Pearson Education, Inc., 2012).
5. C. Kittel, *Introduction to Solid State Physics*, eighth edition (John Wiley & Sons, Inc., 2005).

APPENDIX

I found a very interesting simulation of nuclear magnetic resonance. These youtubes may be useful for your understanding the physics

Youtube:

1. Simple demonstration of magnetic resonance as used in NMR and MRI
<http://www.youtube.com/watch?v=1OrPCNVSA4o>
2. Part 1: Introduction to the Bloch Simulator made for basic MRI and NMR education
<http://www.youtube.com/watch?v=6aWBZtypU7w>

3. Part 2, NMR/MRI-education: Simple spin dynamics explored using the Bloch Simulator

<http://www.youtube.com/watch?v=QaugiVcQ0OE>

4. Part 3, NMR/MRI-education: Spin-echoes explored using the Bloch Simulator

<http://www.youtube.com/watch?v=FxyiH2TjQvI>