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 and γ is the gyromagnetic ratio,

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

μ_p is the nuclear magnetic moment,

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

where μ_N is the nuclear magneton:

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

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 $\boldsymbol{B} = B_0 \, \boldsymbol{e}_z$

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

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

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

f_o (MHz)= $\omega_0/2\pi = 4.258 \, B_0$ (kOe)

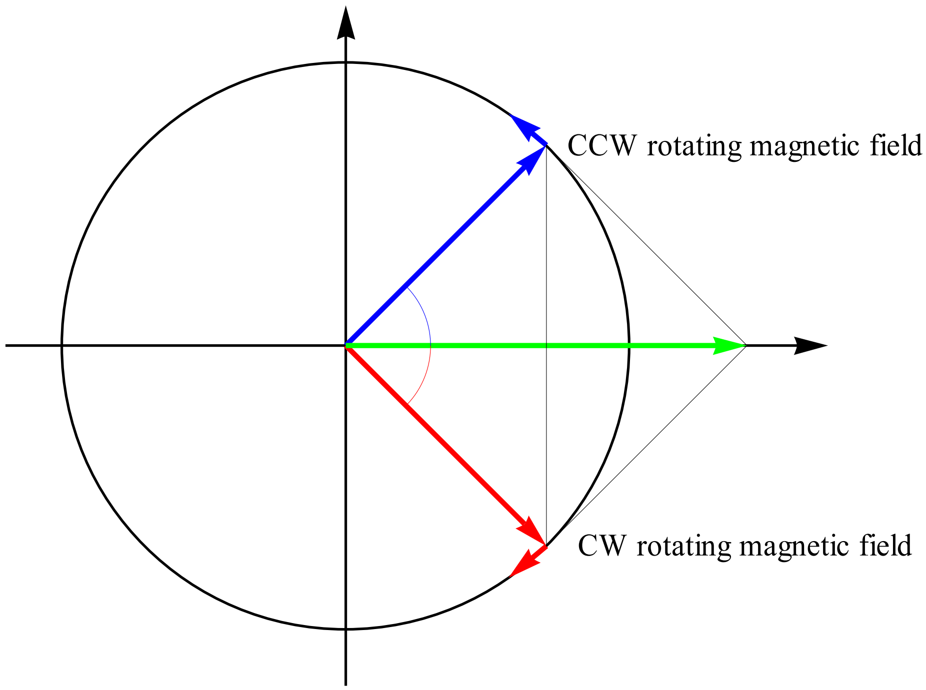
where γ is a gyromagnetic ratio; $\gamma = \frac{\mu_z}{I} = \frac{\mu_z}{\frac{\hbar}{2}\sigma_z}$.

Suppose that

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

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

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



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

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

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

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

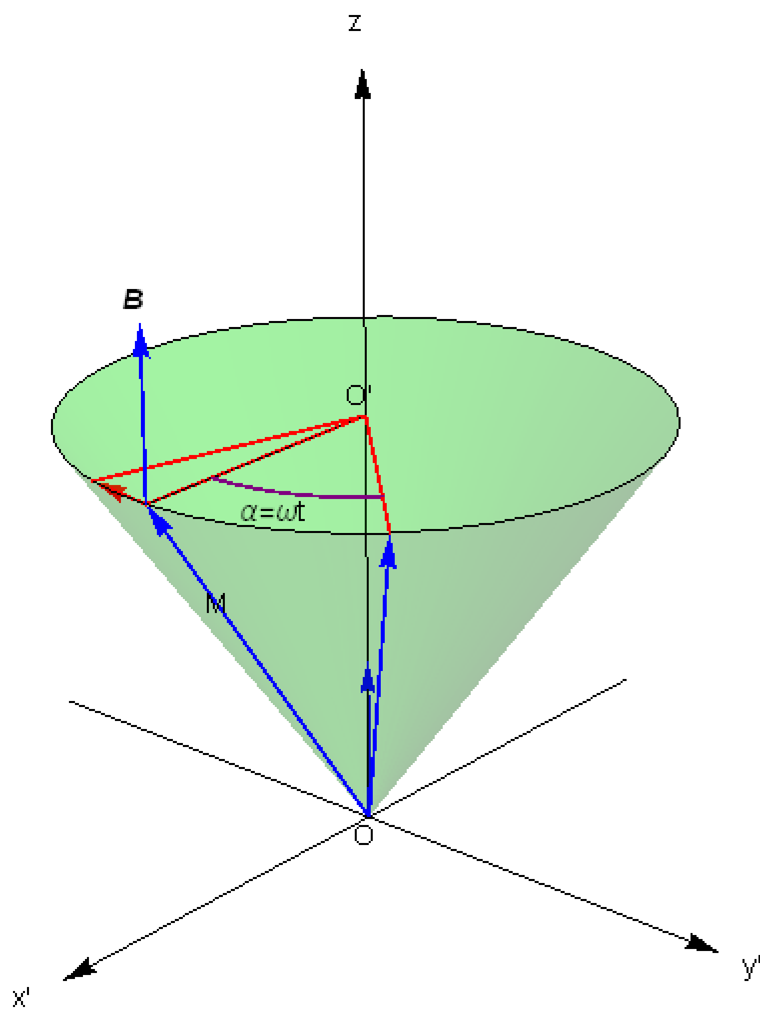


Fig. Larmor precession of the proton magnetic moment in the presence of an external magnetic field $\boldsymbol{B}_0$ along the z axis. The Larmor precession is done in the clockwise direction.

Then Hamiltonian $\hat{H}$ is given by

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

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:

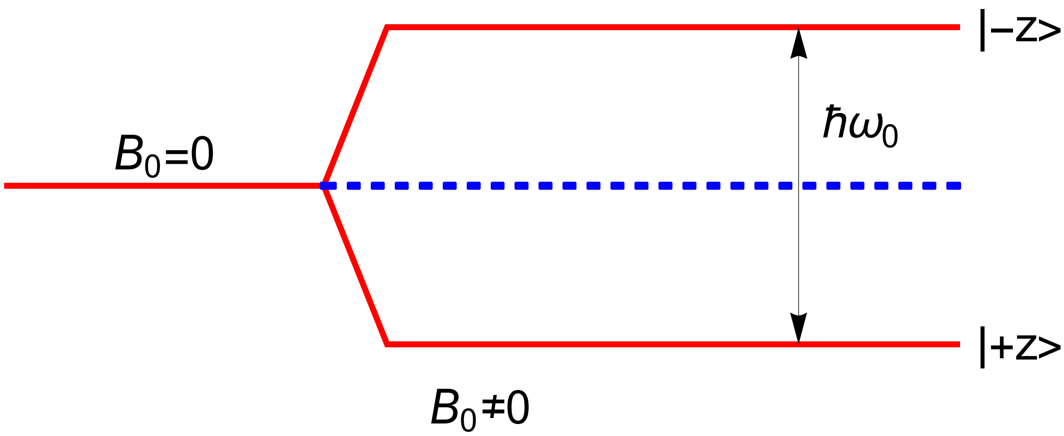
$$|\psi(t)\rangle = \begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} = a_1(t)|+z\rangle + a_2(t)|-z\rangle$$

We use the notations

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

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

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 $\hbar\omega_0$.



The Schrödinger equation is given by

$$i\hbar\frac{\partial}{\partial t}\left|\psi(t)\right\rangle = i\hbar\begin{pmatrix}\frac{da_1}{dt}\\ \frac{da_2}{dt}\end{pmatrix} = \hat{H}\begin{pmatrix}a_1(t)\\ a_2(t)\end{pmatrix} = -\gamma\frac{\hbar}{2}\begin{pmatrix}B_0 & B_1e^{i\omega t}\\ B_1e^{-i\omega t} & -B_0\end{pmatrix}\begin{pmatrix}a_1(t)\\ a_2(t)\end{pmatrix}$$

or

$$\begin{pmatrix}\frac{da_1}{dt}\\ \frac{da_2}{dt}\end{pmatrix} = \frac{i}{2}\begin{pmatrix}\omega_0 & \omega_1e^{i\omega t}\\ \omega_1e^{-i\omega t} & -\omega_0\end{pmatrix}\begin{pmatrix}a_1(t)\\ a_2(t)\end{pmatrix}$$

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

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

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

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

or

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

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

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

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

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

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

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

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

((**Laboratory frame and rotating reference frame**))

We consider the rotation operator

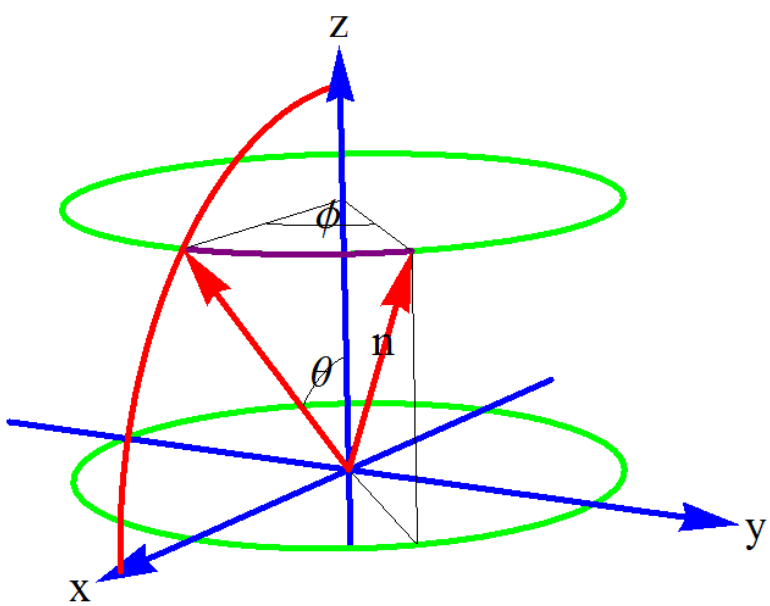
$$|\psi\rangle \to |\psi'\rangle = \hat{R}|\psi\rangle$$

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

$$|\boldsymbol{r}'\rangle = |\Re \boldsymbol{r}\rangle = \hat{R}|\boldsymbol{r}\rangle \qquad \text{for } \boldsymbol{r} \to \boldsymbol{r}' = \Re \boldsymbol{r} .$$

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

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



with

$$\phi = \omega t .$$

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

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

and

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

Note that

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

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

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

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

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

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

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

and

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

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

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

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

where

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

and

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

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

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

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

4. Eigenvalue problem

We can also solve the eigenvaule 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

$$B_{eff}=(B_0-\frac{\omega}{\gamma})\boldsymbol{e}_z+(-B_1)e_x=\frac{\omega_0-\omega}{\gamma}\boldsymbol{e}_z+(-\frac{\omega_1}{\gamma})\boldsymbol{e}_x$$

in the rotating reference frame.

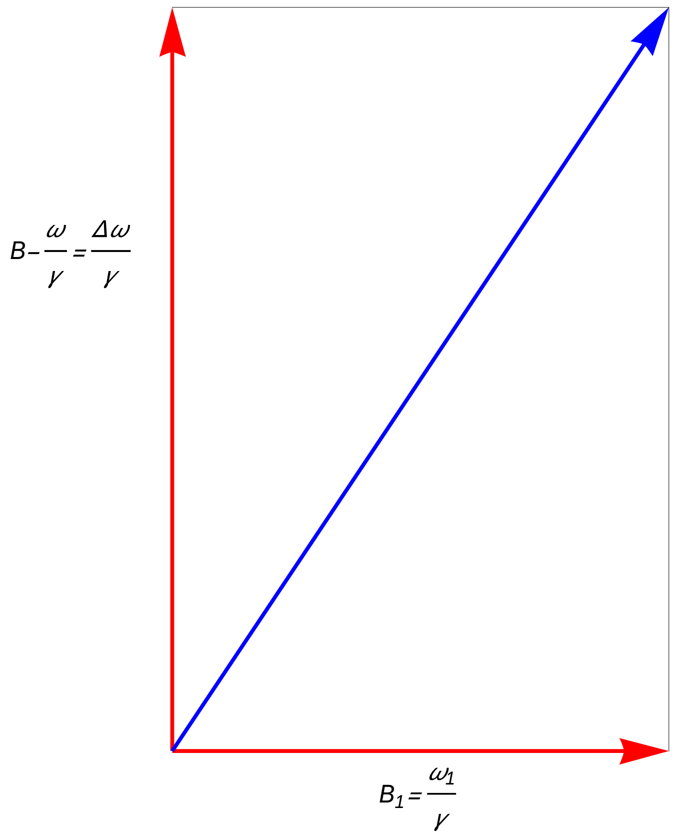


Fig. Effective magnetic field in the rotating reference frame.

or

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

or

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

where

$$(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})\left|\pm\boldsymbol{n}\right\rangle=\pm\left|\pm\boldsymbol{n}\right\rangle$$

or

$$\hat{H}'\left|\pm \boldsymbol{n}\right\rangle = -\frac{\hbar}{2}\sqrt{(\Delta\omega)^2+\omega_1^2}\,(\hat{\boldsymbol{\sigma}}\cdot\boldsymbol{n})\left|\pm \boldsymbol{n}\right\rangle = \mp\frac{\hbar}{2}\sqrt{(\Delta\omega)^2+\omega_1^2}\left|\pm \boldsymbol{n}\right\rangle$$

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

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

with

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

$$\left|+\boldsymbol{n}\right\rangle = \cos\frac{\theta}{2}\left|+z\right\rangle + \sin\frac{\theta}{2}\left|-z\right\rangle$$

$$\left|-\boldsymbol{n}\right\rangle = -\sin\frac{\theta}{2}\left|+z\right\rangle + \cos\frac{\theta}{2}\left|-z\right\rangle$$

where

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

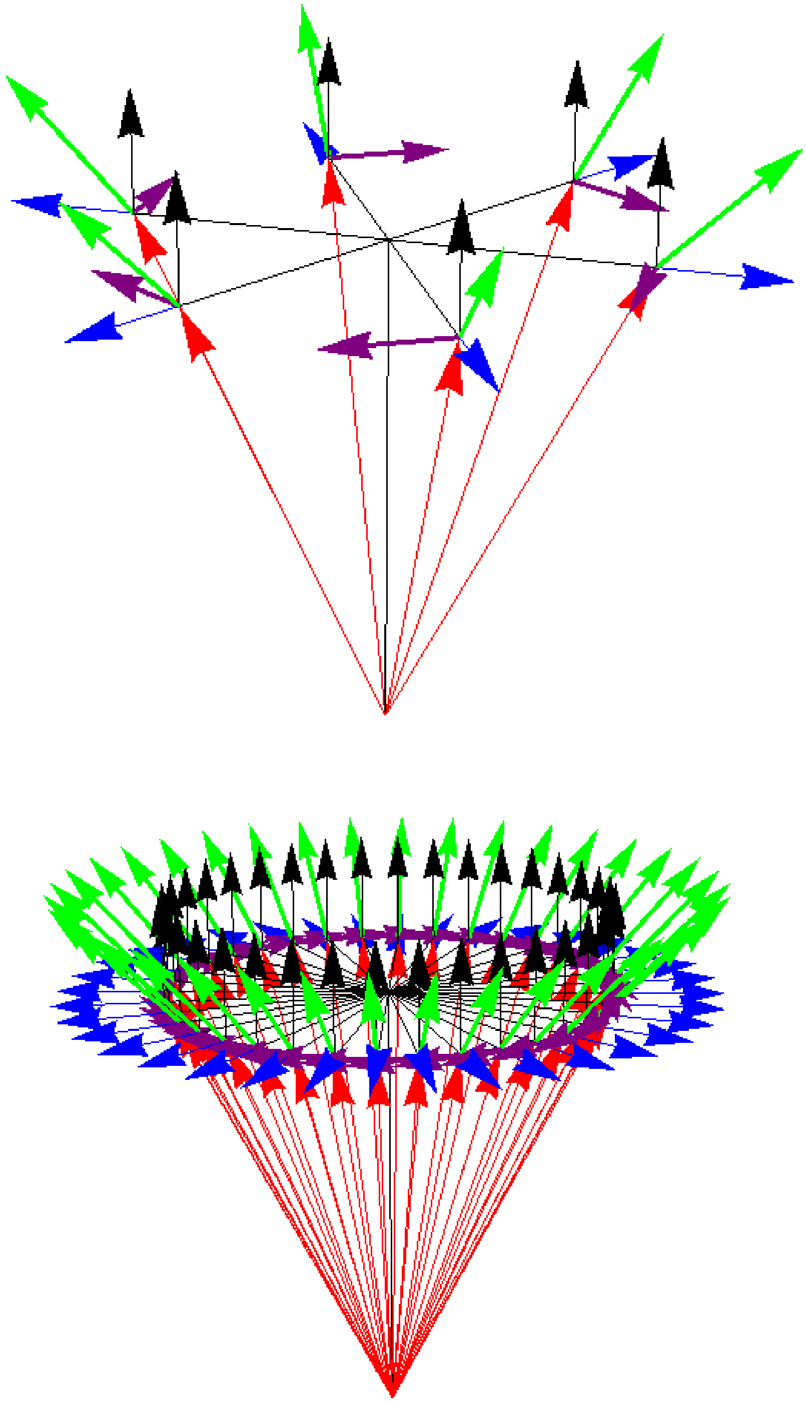


Fig. Red arrow (the nuclear magnetization). Blue arrow (rf magnetic field). Black arrow (the effective magnetic field along the z axis). Green arrow (the resultant effective magnetic field). The purple arrow (the torque).

5. Rabi's formula

We assume that the initial condition is given by

$$\left|\psi'(t=0)\right\rangle = \left|\psi(t=0)\right\rangle = \left|+z\right\rangle \qquad \text{(initial condition)}$$

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

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

or

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

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

Then we have

$$\left|\psi'(t)\right\rangle = \left|+z\right\rangle\left\langle +z\middle|\psi'(t)\right\rangle + \left|-z\right\rangle\left\langle -z\middle|\psi'(t)\right\rangle$$
$$= [\cos(\tfrac{\Omega}{2}t) + i\cos\theta\sin(\frac{\Omega}{2}t)]\left|+z\right\rangle + i\sin\theta\sin(\frac{\Omega}{2}t)\left|-z\right\rangle$$

and

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

The Rabi's formula:

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

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

$$P_-(t) = \left|\left\langle -z\middle|\psi(t)\right\rangle\right|^2 = \left|\left\langle -z\middle|\psi'(t)\right\rangle\right|^2$$
$$= \sin^2\theta\sin^2(\frac{\Omega t}{2})$$
$$= \sin^2\theta\sin^2(\frac{t}{2}\sqrt{(\Delta\omega)^2 + \omega_1^2})$$
$$= \frac{\omega_1{}^2}{(\Delta\omega)^2 + \omega_1^2}\sin^2(\frac{t}{2}\sqrt{(\Delta\omega)^2 + \omega_1^2})$$

$$P_+(t) = \left|\left\langle -z\middle|\psi(t)\right\rangle\right|^2 = \left|\left\langle -z\middle|\psi'(t)\right\rangle\right|^2 = \cos^2(\frac{\Omega}{2}t) + \cos^2\theta\sin^2(\frac{\Omega}{2}t)]$$

with

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

((**Note**))

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

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

Then we have

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

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

or

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

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

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 = ℏ/2 ( Δω  -ω1 ; -ω1  -Δω ); M1 = MatrixExp[-ⅈ/ℏ H1 t] // FullSimplify;
rule1 = {Sqrt[-Δω^2 - ω1^2] → ⅈ Ω, 1/Sqrt[-Δω^2 - ω1^2] → -ⅈ/Ω};
M2 = M1 /. rule1 // Simplify
```

$$\left\{\left\{\text{Cos}\left[\frac{t\,\Omega}{2}\right] - \frac{i\,\Delta\omega\,\text{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega}, \frac{i\,\omega 1\,\text{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega}\right\}, \left\{\frac{i\,\omega 1\,\text{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega}, \text{Cos}\left[\frac{t\,\Omega}{2}\right] + \frac{i\,\Delta\omega\,\text{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega}\right\}\right\}$$

P11: Probabilityof finding in the state |+z >
P21: Probability of finding in the state |-z>
with

$$\sqrt{\Delta\omega^2 + \omega 1^2} = \Omega$$

```
P1 = {1, 0}.M2.{1, 0} // Simplify; P11 = P1* P1 // Simplify
```

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

```
P2 = {0, 1}.M2.{1, 0} // Simplify; P21 = P2* P2 // Simplify
```

$$\frac{\omega 1^2\,\mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]^2}{\Omega^2}$$

6. Summary

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

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

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

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

where

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

We assume that

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

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

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

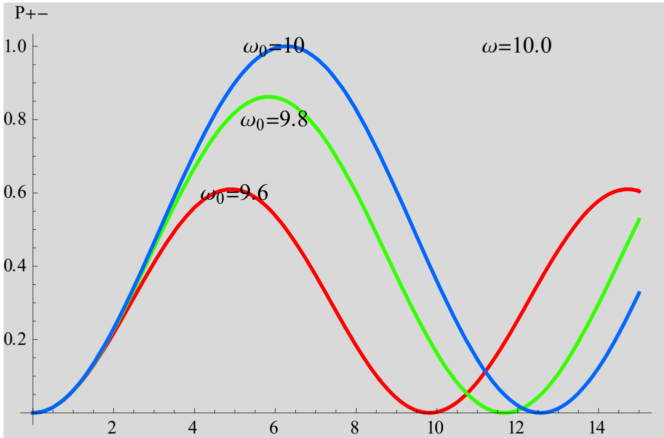


Fig. $P_- = P_-$ vs t. $\omega_1 = 0.5$. $\omega = 10$. ω_0 is changed as a parameter.

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

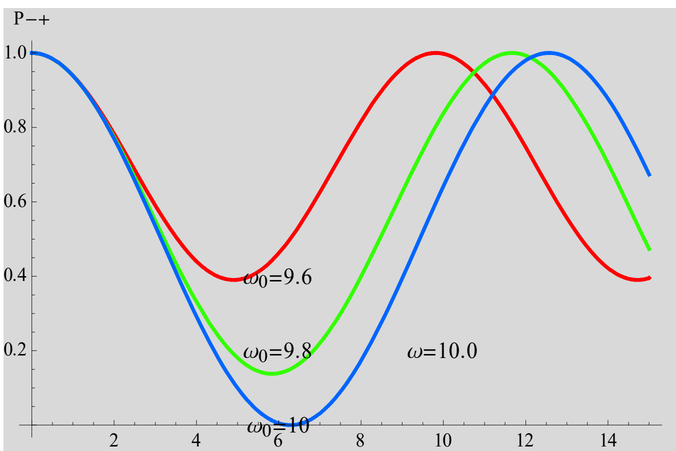


Fig. P_+ vs t. $\omega_1 = 0.5$. $\omega = 10$. ω_0 is changed as a parameter.

The state vector is given by

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

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

7. Expectation values

The expectation value

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

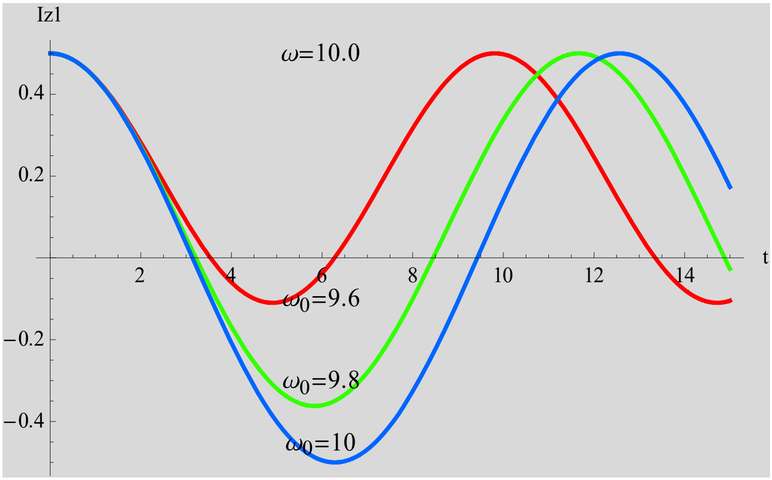


Fig. $\langle I_z \rangle$ vs t. $\omega_1 = 0.5$. $\omega = 10$. ω_0 is changed as a parameter.

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

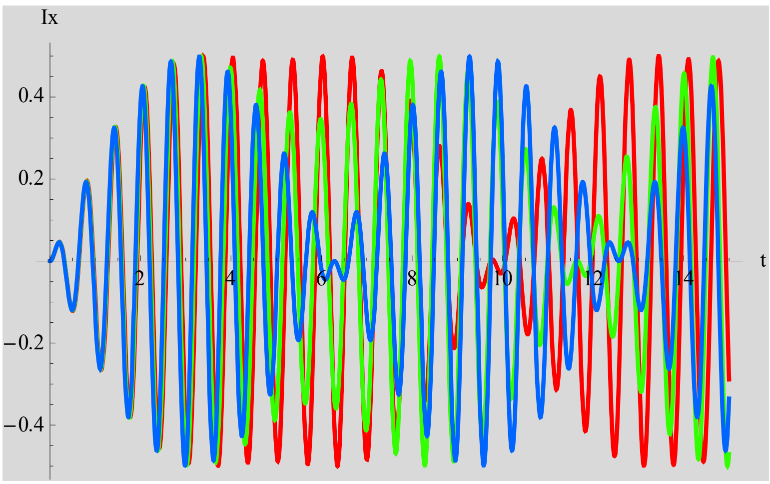


Fig. $\langle I_x \rangle$ vs t. $\omega_1 = 0.5$. $\omega = 10$. ω_0 is changed as a parameter.

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

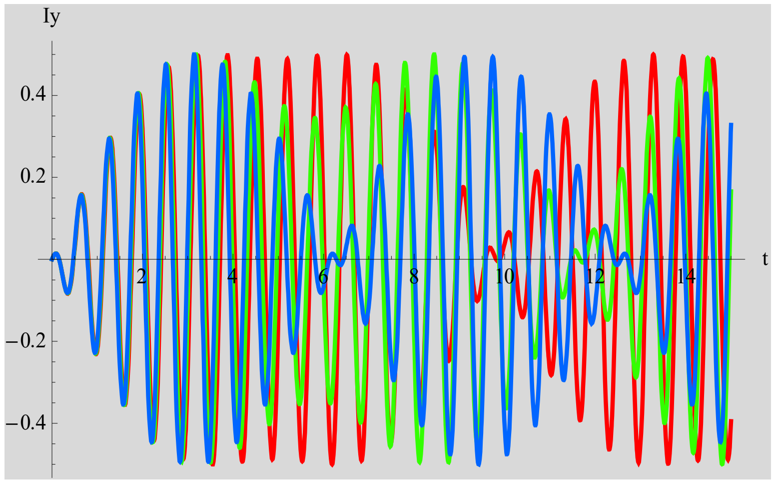


Fig. $<I_y>$ vs t. $\omega_1 = 0.5$. $\omega = 10$. ω_0 is changed as a parameter.

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

In Townsend book, the magnetic field is given by

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

leading to

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

In the present case we assume that

$\boldsymbol{B}_1 = 2\, B_1 \cos(\omega t)\, \boldsymbol{e}_x$ (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

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

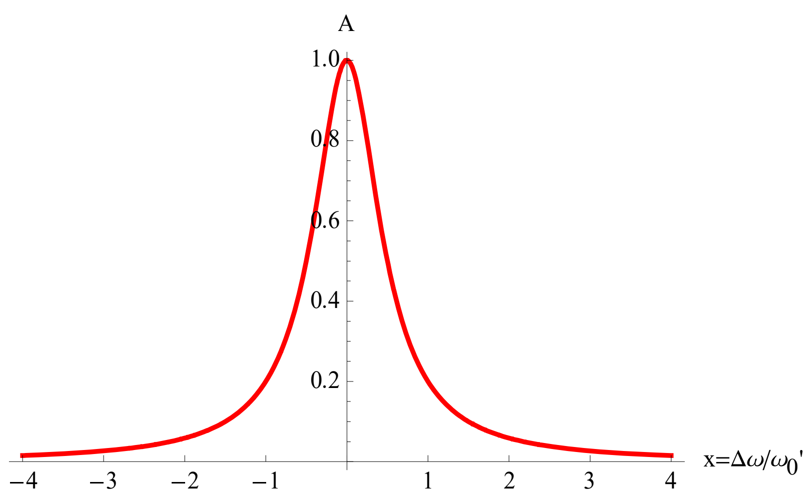
The probability is

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

(Rabi's formula in Townsend book). The amplitude of $P_{+\to-}(t)$ 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]};
```

$$H1 = \frac{\hbar}{2}\{\{\Delta\omega, -\omega 1\}, \{-\omega 1, -\Delta\omega\}\};\ \sigma x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix};\ \sigma y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix};$$

$$\sigma z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix};\ rule1 = \left\{\sqrt{-\Delta\omega^2 - \omega 1^2} \to i\,\Omega,\ \frac{1}{\sqrt{-\Delta\omega^2 - \omega 1^2}} \to -i\frac{1}{\Omega}\right\};$$

$$rule2 = \left\{\Omega \to \sqrt{\Delta\omega^2 + \omega 1^2},\ \Delta\omega \to (\omega - \omega 0),\ \omega 1 \to 0.5,\ \omega \to 10\right\};$$

$$A1 = MatrixExp\left[\frac{i}{2}\,\omega\, t\, \sigma z\right].MatrixExp\left[-\frac{i}{\hbar}\, H1\, t\right]\ /.\ rule1\ //\ FullSimplify;$$

```
ψ1 = A1.{1, 0} // ComplexExpand // FullSimplify
```

$$\left\{\frac{e^{\frac{i t \omega}{2}}\left(\Omega \operatorname{Cos}\left[\frac{t\Omega}{2}\right] - i\,\Delta\omega \operatorname{Sin}\left[\frac{t\Omega}{2}\right]\right)}{\Omega},\ \frac{i\, e^{-\frac{1}{2} i t \omega}\,\omega 1 \operatorname{Sin}\left[\frac{t\Omega}{2}\right]}{\Omega}\right\}$$

$$Ix = \frac{1}{2}\,\psi 1^{*}.\sigma x.\psi 1\ //\ ComplexExpand\ //\ FullSimplify$$

$$\frac{\omega 1\left(-2\,\Delta\omega \operatorname{Cos}[t\,\omega] \operatorname{Sin}\left[\frac{t\Omega}{2}\right]^2 + \Omega \operatorname{Sin}[t\,\omega] \operatorname{Sin}[t\,\Omega]\right)}{2\,\Omega^2}$$

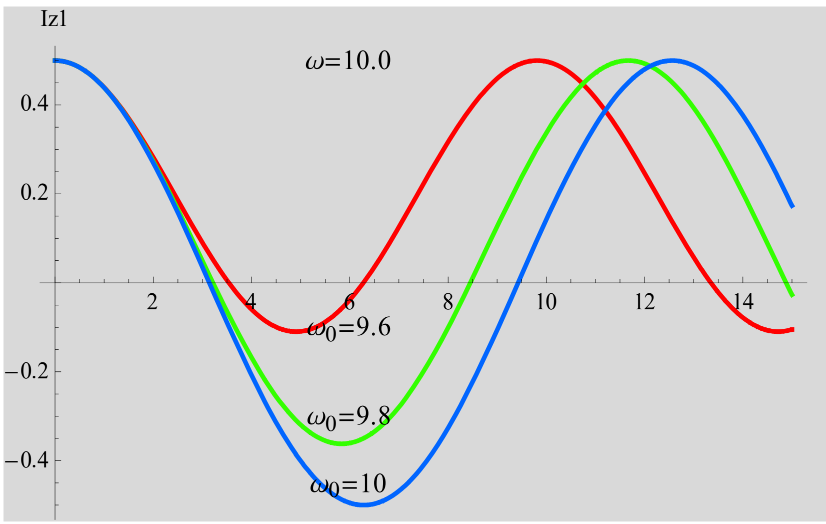
$$Iy = \frac{1}{2}\,\psi 1^{*}.\sigma y.\psi 1\ //\ FullSimplify$$

$$\frac{\Delta\omega\,\omega 1 \operatorname{Sin}[t\,\omega] \operatorname{Sin}\left[\frac{t\Omega}{2}\right]^2 + \frac{1}{2}\,\Omega\,\omega 1 \operatorname{Cos}[t\,\omega] \operatorname{Sin}[t\,\Omega]}{\Omega^2}$$

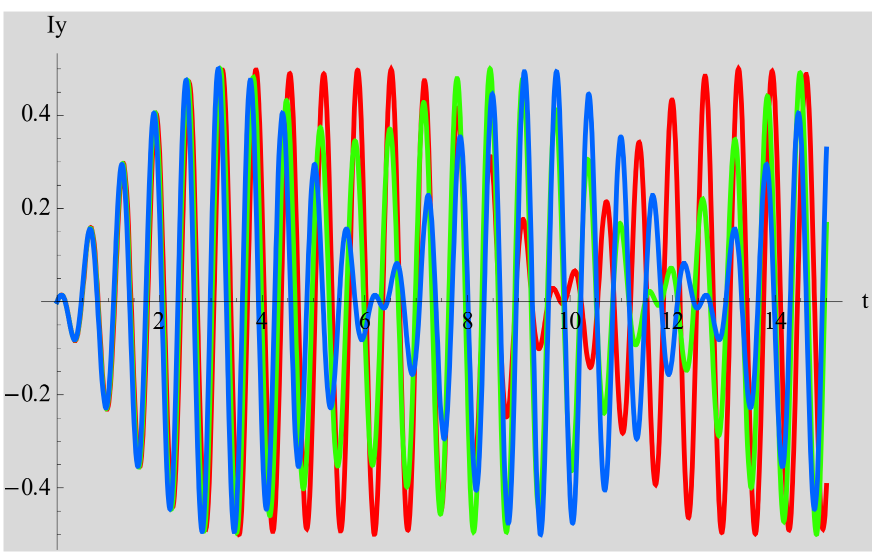
$$Iz = \frac{1}{2}\,\psi 1^{*}.\sigma z.\psi 1\ //\ ComplexExpand\ //\ FullSimplify$$

$$\frac{1}{2}\left(\operatorname{Cos}\left[\frac{t\,\Omega}{2}\right]^2 + \frac{(\Delta\omega - \omega 1)\,(\Delta\omega + \omega 1) \operatorname{Sin}\left[\frac{t\Omega}{2}\right]^2}{\Omega^2}\right)$$

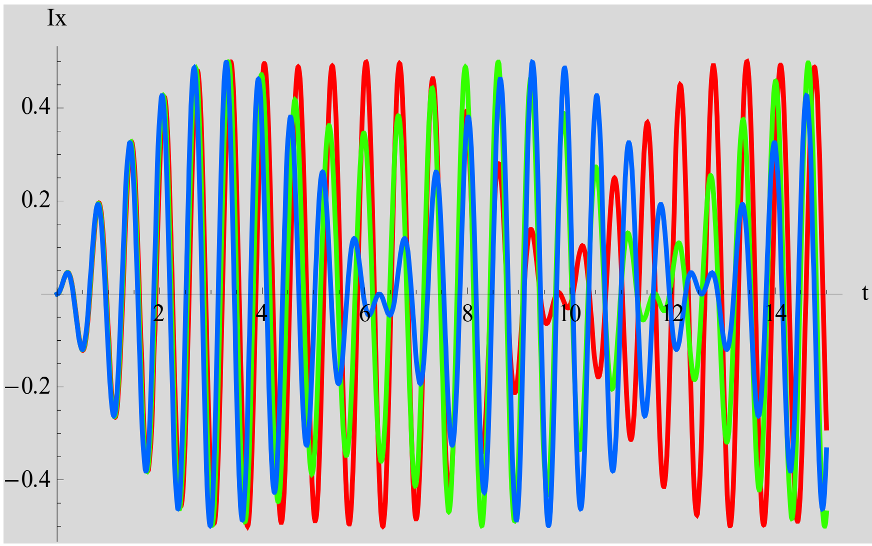
```
Iz1 = Iz //. rule2;
k1 = Plot[Evaluate[Table[Iz1, {ω0, 9.6, 10, 0.2}]], {t, 0, 15},
  PlotStyle → Table[{Thick, Hue[0.3 i]}, {i, 0, 20}],
  Background → LightGray, AxesLabel → {"t", "Iz1"}, PlotRange → All];
k2 = Graphics[{Text[Style["ω0=10", Black, 12], {6, -0.45}],
   Text[Style["ω0=9.8", Black, 12], {6, -0.30}],
   Text[Style["ω0=9.6", Black, 12], {6, -0.1}],
   Text[Style["ω=10.0", Black, 12], {6, 0.5}]}];
Show[k1, k2]
```




```
Iy1 = Iy //. rule2;
p1 = Plot[Evaluate[Table[Iy1, {ω0, 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]
```

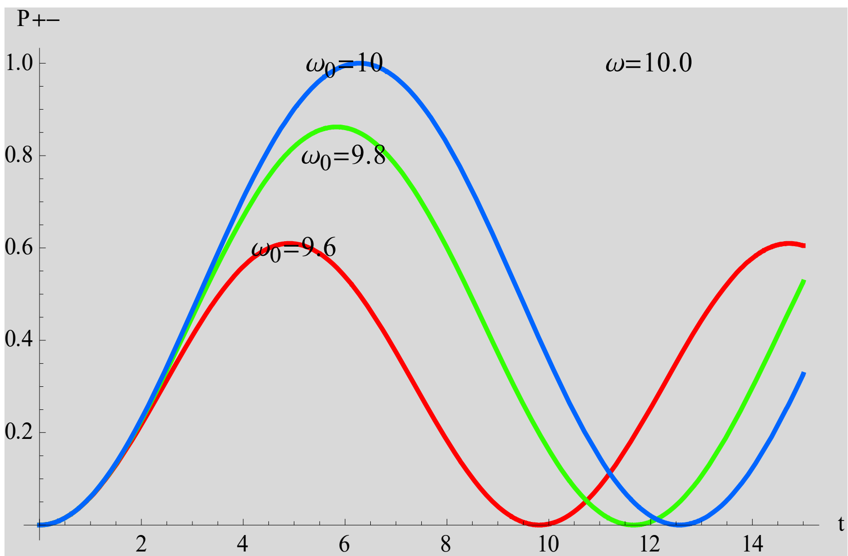


```
Ix1 = Ix //. rule2;
p2 = Plot[Evaluate[Table[Ix1, {ω0, 9.6, 10, 0.2}]], {t, 0, 15},
  PlotStyle → Table[{Thick, Hue[0.3 i]}, {i, 0, 20}],
  Background → LightGray, AxesLabel → {"t", "Ix"}, PlotRange → All]
```

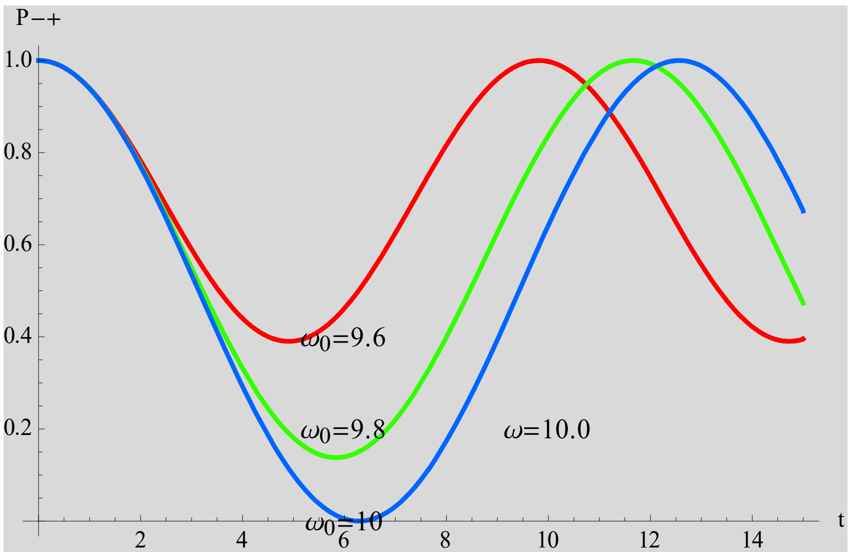


```
B1 = MatrixExp[-(i/ħ) H1 t] /. rule1 // FullSimplify; P1 = {0, 1}.B1.{1, 0};
P11 = Abs[P1]^2;
P12 = P11 //. rule2;

h1 = Plot[Evaluate[Table[P12, {ω0, 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["ω0=10", Black, 12], {6, 1}],
   Text[Style["ω0=9.8", Black, 12], {6, 0.8}],
   Text[Style["ω0=9.6", Black, 12], {5, 0.6}],
   Text[Style["ω=10.0", Black, 12], {12, 1}]}];
Show[h1, h2]
```



```
h3 = Plot[Evaluate[Table[1 - P12, {ω0, 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["ω0=10", Black, 12], {6, 0}],
   Text[Style["ω0=9.8", Black, 12], {6, 0.2}],
   Text[Style["ω0=9.6", Black, 12], {6, 0.4}],
   Text[Style["ω=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
```

$$\left\{\frac{1}{2} e^{\frac{i t \omega}{2}} (i (\omega - \omega 0) b1[t] - i \omega 1 b2[t] + 2 b1'[t]),\right.$$
$$\left. -\frac{1}{2} i e^{-\frac{1}{2} i t \omega} (\omega 1 b1[t] + (\omega - \omega 0) b2[t] + 2 i b2'[t])\right\}$$

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

$$\left\{\left\{b1'[t] \to \frac{1}{2} i ((-\omega + \omega 0) b1[t] + \omega 1 b2[t])\right\}\right\}$$

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

$$\left\{\left\{b2'[t] \to \frac{1}{2} i (\omega 1 b1[t] + (\omega - \omega 0) b2[t])\right\}\right\}$$

New matrix

$$NM = \left\{\left\{\frac{1}{2} i (\omega 0 - \omega), \frac{1}{2} i \omega 1\right\}, \left\{\frac{1}{2} i \omega 1, \frac{1}{2} i (\omega - \omega 0)\right\}\right\};$$

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

$$rule2 = \left\{\sqrt{-\omega^2 + 2 \omega \omega 0 - \omega 0^2 - \omega 1^2} \to i \Omega, \frac{1}{\sqrt{-\omega^2 + 2 \omega \omega 0 - \omega 0^2 - \omega 1^2}} \to -i \frac{1}{\Omega}\right\};$$

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

$$\left\{\left\{\frac{\Omega\,\mathrm{Cos}\left[\frac{t\,\Omega}{2}\right]-i\,(\omega-\omega 0)\,\mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega},\ \frac{i\,\omega 1\,\mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega}\right\},\ \left\{\frac{i\,\omega 1\,\mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega},\ \frac{\Omega\,\mathrm{Cos}\left[\frac{t\,\Omega}{2}\right]+i\,(\omega-\omega 0)\,\mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega}\right\}\right\}$$

```
ψ1 = EE.{1, 0} // Simplify
```

$$\left\{\frac{\Omega\,\mathrm{Cos}\left[\frac{t\,\Omega}{2}\right]-i\,(\omega-\omega 0)\,\mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega},\ \frac{i\,\omega 1\,\mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega}\right\}$$

```
C1 = ψ1[[1]]
```

$$\frac{\Omega\,\mathrm{Cos}\left[\frac{t\,\Omega}{2}\right]-i\,(\omega-\omega 0)\,\mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega}$$

```
C2 = ψ1[[2]]
```

$$\frac{i\,\omega 1\,\mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega}$$

```
rule3 = {ω^2 - 2 ω ω0 + ω0^2 → Ω^2 - ω1^2};

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

$$\frac{\omega^2+\Omega^2-2\,\omega\,\omega 0+\omega 0^2-\left(\omega^2-\Omega^2-2\,\omega\,\omega 0+\omega 0^2\right)\mathrm{Cos}[t\,\Omega]}{2\,\Omega^2}$$

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

$$\frac{\omega 1^2 \, \mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]^2}{\Omega^2}$$

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

1

The final result is as follows.

$$P2 = \frac{\omega 1^2 \, \mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]^2}{\Omega^2} \text{ and } P1 = 1 - P2 \, *)$$

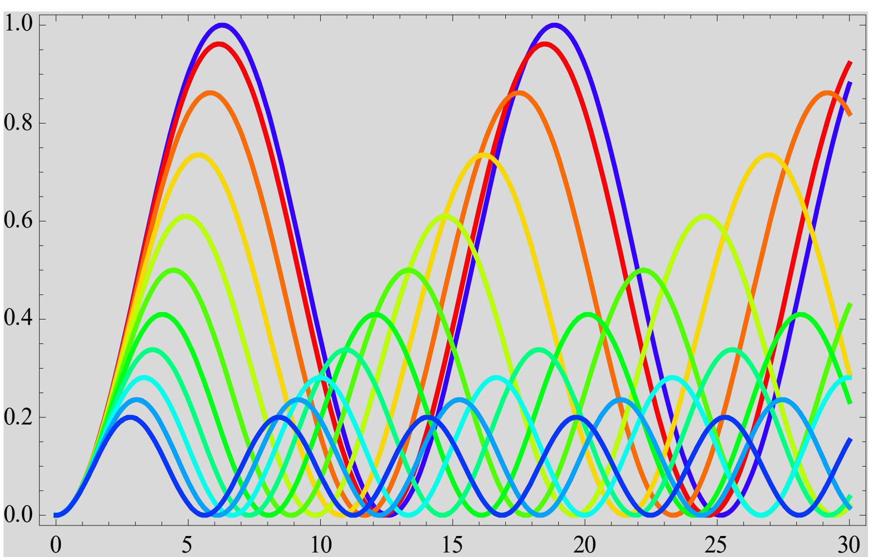
```
rule5 = {Ω → Sqrt[ω^2 - 2 ω ω0 + ω0^2 + ω1^2]};

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

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

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

The Hamiltonian $\hat{H}$ is given by

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

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

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

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

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

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

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

and

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

$$= -\frac{1}{2}\hbar\omega_1 \begin{pmatrix} e^{-i\omega_0 t/2} & 0 \\ 0 & e^{i\omega_0 t/2} \end{pmatrix} \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix} \begin{pmatrix} e^{i\omega_0 t/2} & 0 \\ 0 & e^{-i\omega_0 t/2} \end{pmatrix}$$

$$= -\frac{1}{2}\hbar\omega_1 \begin{pmatrix} 0 & e^{i(\omega-\omega_0)t} \\ e^{-i(\omega-\omega_0)t} & 0 \end{pmatrix}$$

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

We assume the wave function:

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

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

where

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

or

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

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.

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

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

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

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

The probability:

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

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

((**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] == (I/2) ω1 Exp[I Δ t] b2[t];

eq2 = D[b2[t], t] == (I/2) ω1 Exp[-I Δ t] b1[t];

s11 = DSolve[{eq1, eq2, b1[0] == 1, b2[0] == 0},
    {b1[t], b2[t]}, t] // Simplify[#, {Δ > 0, ω1 > 0}] &;

s12 = s11 /. {Sqrt[ω1^2 + Δ^2] -> Ω, 1/Sqrt[ω1^2 + Δ^2] -> 1/Ω} // Simplify;

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

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

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

$$\frac{i\, e^{-\frac{1}{2} i\, t\, \Delta}\, \omega 1\, \mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]}{\Omega}$$

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

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

```
P11 = P1 /. {Ω → Sqrt[ω1^2 + Δ^2]} // Simplify
```

$$\frac{2\,\Delta^2 + \omega 1^2 + \omega 1^2\, \mathrm{Cos}\left[t\sqrt{\Delta^2 + \omega 1^2}\right]}{2\left(\Delta^2 + \omega 1^2\right)}$$

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

$$\frac{\omega 1^2\, \mathrm{Sin}\left[\frac{t\,\Omega}{2}\right]^2}{\Omega^2}$$

```
P21 = P2 /. {Ω → Sqrt[ω1^2 + Δ^2]} // Simplify
```

$$\frac{\omega 1^2 \,\text{Sin}\left[\frac{1}{2}\, t \sqrt{\Delta^2 + \omega 1^2}\right]^2}{\Delta^2 + \omega 1^2}$$

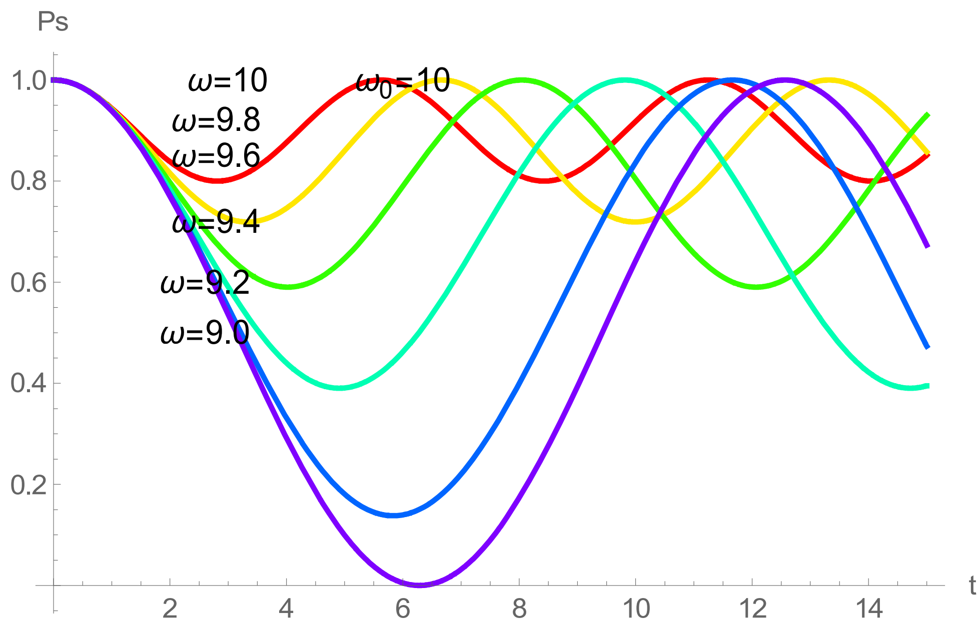
```
P11 + P21 // Simplify
```

1

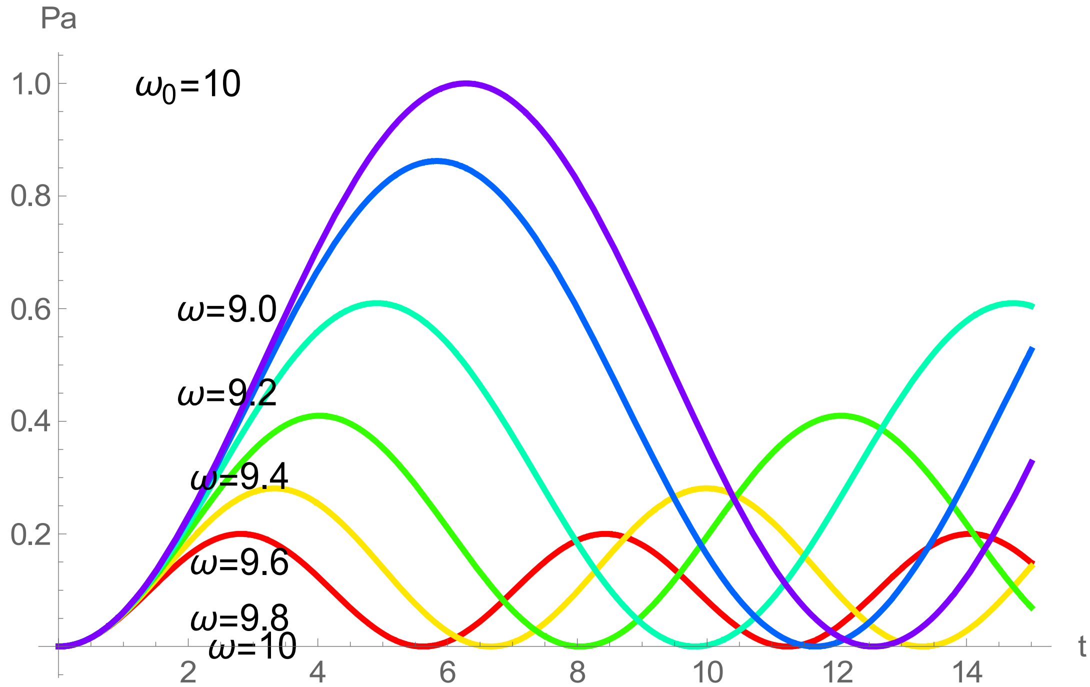
```
ga11 = P11 //. {Δ → ω - ω0, ω0 → 10, ω1 → 0.5}
```

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

```
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, {ω, 9, 10, 0.2}]],
   {t, 0, 15},
   PlotStyle → Table[{Thick, Hue[0.15 i]}, {i, 0, 5}],
   AxesLabel → {"t", "Pa"}];
f2 = Graphics[{Text[Style["ω0=10", Black, 12], {2, 1}],
    Text[Style["ω=10", Black, 12], {3, 0}],
    Text[Style["ω=9.8", Black, 12], {2.8, 0.05}],
    Text[Style["ω=9.6", Black, 12], {2.8, 0.15}],
    Text[Style["ω=9.4", Black, 12], {2.8, 0.3}],
    Text[Style["ω=9.2", Black, 12], {2.6, 0.45}],
    Text[Style["ω=9.0", Black, 12], {2.6, 0.6}]}];
Show[f1, f2]
```



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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 very intersting 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