Chapter 29S
Maser and laser physics, and magnetic resonance
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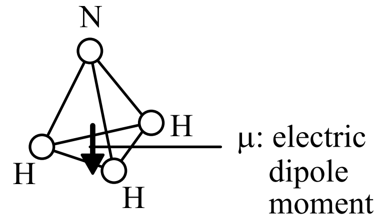
Maser
Laser
Rabi's formula
Rotating wave approximation
Nuclear magnetic resonance

Isidor Isaac Rabi (29 July 1898 – 11 January 1988) was a Galician-born American physicist and Nobel laureate recognized in 1944 for his discovery of nuclear magnetic resonance.

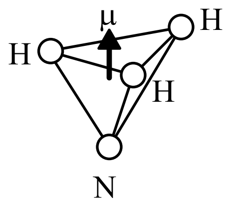
http://en.wikipedia.org/wiki/Isidor_Isaac_Rabi

29S.1 Maser

A maser is a device that produces coherent electromagnetic waves through amplification due to stimulated emission. Historically the term came from the acronym "microwave amplification by stimulated emission of radiation", although modern masers emit over a broad portion of the electromagnetic spectrum. This has led some to replace "microwave" with "molecular" in the acronym, as suggested by Townes. When optical coherent oscillators were first developed, they were called optical masers, but it has become more common to refer to these as lasers.



$|1\rangle$ when the nitrogen is up.



$|2\rangle$ when the nitrogen is down.

We consider the parity operator $\hat{\pi}$, such that

$$\hat{\pi}|1\rangle = |2\rangle \qquad\qquad \hat{\pi}|2\rangle = |1\rangle$$

Therefore the kets $|1\rangle$ and $|2\rangle$ are not the eigenkets of $\hat{\pi}$. Since

$$\hat{\pi} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$\hat{\pi}$ is regarded as the Pauli matrix $\hat{\sigma}_x$. The eigenkets of $\hat{\sigma}_x$ are $|\pm\rangle_x$.

$$\hat{\sigma}_x|\pm\rangle_x = \pm|\pm\rangle_x$$

with

$$|+\rangle_x = \left|\varphi_s^{(0)}\right\rangle = \frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)\text{; symmetric state.}$$

$$|-\rangle_x = \left|\varphi_A^{(0)}\right\rangle = \frac{1}{\sqrt{2}}(|1\rangle - |2\rangle)\text{; antisymmetric state}$$

These two states are the eigenkets of $\hat{\pi}$. We now consider the Hamiltonain $\hat{H}$. The symmetry of two physical configuration suggests that

$$\langle 1|\hat{H}|1\rangle = \langle 2|\hat{H}|2\rangle = E_0$$

What about the off-diagonal elements? The vanishing of $\langle 2|\hat{H}|1\rangle$ would mean that a molecule initially in the state $|1\rangle$ would remain in that state. If $\langle 2|\hat{H}|1\rangle \neq 0$, there is a small amplitude for the system to mix between the two states.

$$\langle 2|\hat{H}|1\rangle = -A$$

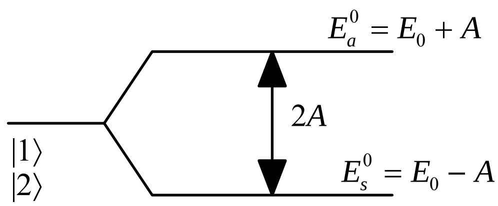
$$\hat{H} = \begin{pmatrix} E_0 & -A \\ -A & E_0 \end{pmatrix} = E_0\hat{1} - A\hat{\sigma}_x$$

This Hamiltonian commutates with the parity operator: $[\hat{H},\hat{\pi}] = \hat{0}$.

$$\hat{\sigma}_x|\pm\rangle_x = \pm|\pm\rangle_x$$

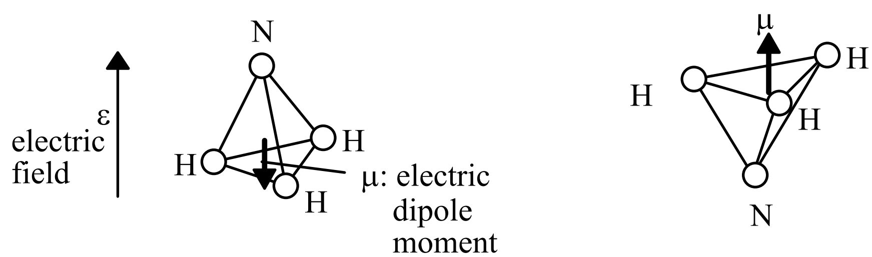
Eigenvalue problem

$$\hat{H}|\pm\rangle_x = (E_0\hat{1} - A\hat{\sigma}_x)|\pm\rangle_x = (E_0 \mp A)|\pm\rangle_x$$



A°0 (perturbation)

29S.2 Application of electric field



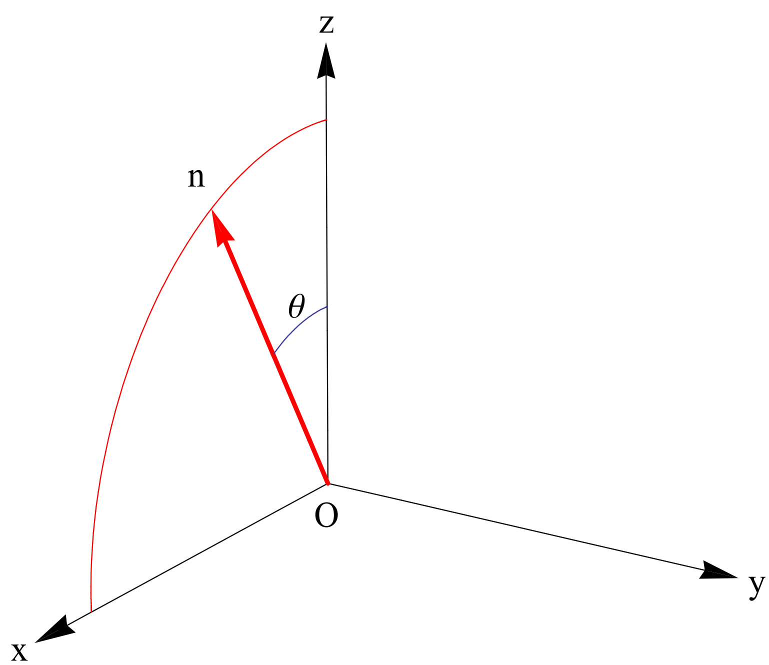
energy = με   energy = -με

When the electric filed is applied along the x axis (the axis of the electric dipole moment), the Hamiltonian is changed into

$$\hat{H} = \begin{pmatrix} E_0 + \mu\varepsilon & -A \\ -A & E_0 - \mu\varepsilon \end{pmatrix} = E_0\hat{1} + \mu\varepsilon\hat{\sigma}_z - A\hat{\sigma}_x$$

The new Hamiltonian $\hat{H}$ does not commutate with the parity operator $\hat{\pi}$.

$$\hat{H} = E_0 \hat{1} + \sqrt{(\mu\varepsilon)^2 + A^2}\,(-\frac{A}{\sqrt{(\mu\varepsilon)^2 + A^2}}\hat{\sigma}_x + \frac{\mu\varepsilon}{\sqrt{(\mu\varepsilon)^2 + A^2}}\hat{\sigma}_z$$



$$\mathbf{n} = (-\frac{A}{\sqrt{(\mu\varepsilon)^2 + A^2}}, 0, \frac{\mu\varepsilon}{\sqrt{(\mu\varepsilon)^2 + A^2}})$$

$$\hat{H} = E_0 \hat{1} + \sqrt{(\mu\varepsilon)^2 + A^2}\,\hat{\sigma}\cdot\mathbf{n}$$

$$\hat{\sigma}\cdot\mathbf{n}\left|\pm\right\rangle_n = \pm\left|\pm\right\rangle_n$$

where

$$\left|+\right\rangle_n = \cos\frac{\theta}{2}\left|1\right\rangle + \sin\frac{\theta}{2}\left|2\right\rangle$$

and

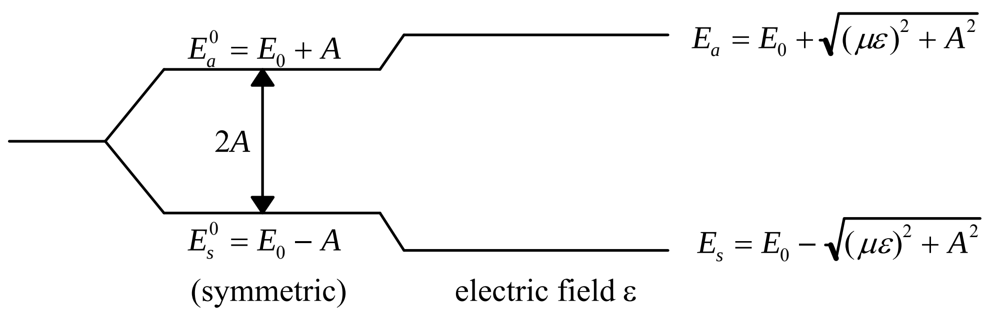
$$|-\rangle_n = -\sin\frac{\theta}{2}|1\rangle + \cos\frac{\theta}{2}|2\rangle$$

where

$$\sin\theta = -\frac{A}{\sqrt{(\mu\varepsilon)^2 + A^2}} \qquad\qquad \cos\theta = \frac{\mu\varepsilon}{\sqrt{(\mu\varepsilon)^2 + A^2}}$$

Thus we have

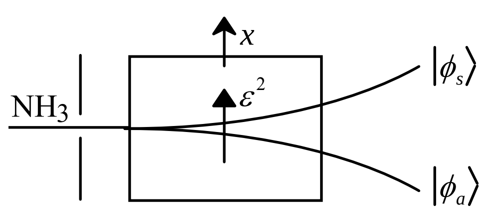
$$\hat{H}|\pm\rangle_n = (E_0 \pm \sqrt{(\mu\varepsilon)^2 + A^2})|\pm\rangle_n$$



In a weak electric field

$$E_s = E_0 - A\sqrt{1 + \frac{\mu^2\varepsilon^2}{A^2}} = E_0 - A - \frac{\mu^2\varepsilon^2}{2A^2} + ...$$

$$E_a = E_0 + A\sqrt{1 + \frac{\mu^2\varepsilon^2}{A^2}} = E_0 + A + \frac{\mu^2\varepsilon^2}{2A^2} + ...$$



Let us consider NH_3 in a region where ε is weak but where ε^2 has a strong gradient in the x-direction (i.e., along the axis of molecules).

$$\frac{d}{dx}(\varepsilon^2) = \lambda .$$

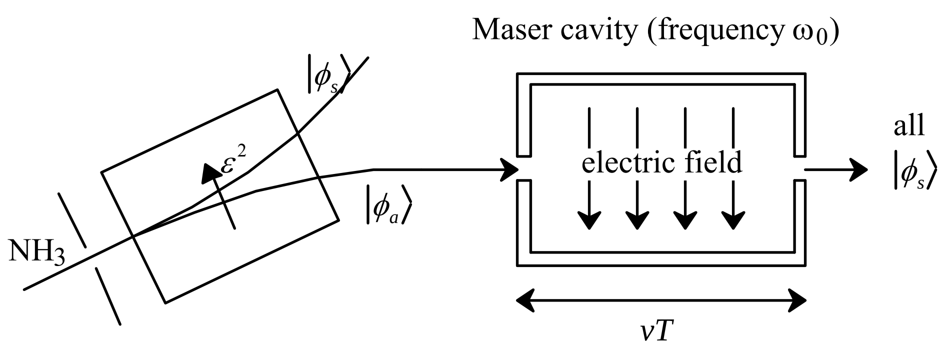
The molecules in the state $|\varphi_s\rangle$ are subjected to a force parallel to the x axis:

$$F_s = -\frac{dE_s}{dx} = \frac{1}{2}\lambda\frac{\mu^2}{A}$$

Similarly, the molecules in the state $|\varphi_a\rangle$ are subjected to an opposite force:

$$F_a = -\frac{dE_a}{dx} = -\frac{1}{2}\lambda\frac{\mu^2}{A}$$

This is the basis of the method which is used in the ammonia maser to sort the molecules and select those in the higher energy state.



In the ammonia maser, the beam with molecules in the state $|\varphi_a^{(0)}\rangle$ and with the higher energy is sent through a resonant cavity.

$$|\psi(t)\rangle = c_1(t)|1\rangle + c_2(t)|2\rangle = c_a(t)|\varphi_a^{(0)}\rangle + c_s(t)|\varphi_s^{(0)}\rangle$$

or

$$\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \begin{pmatrix} \dfrac{c_a(t)+c_s(t)}{\sqrt{2}} \\ \dfrac{-c_a(t)+c_s(t)}{\sqrt{2}} \end{pmatrix} = \begin{pmatrix} \dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{2}} \\ -\dfrac{1}{\sqrt{2}} & \dfrac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} c_a(t) \\ c_s(t) \end{pmatrix}$$

or

Schrödinger equation

$$i\hbar \frac{d}{dt}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix} = \begin{pmatrix} E_0 + \mu\varepsilon(t) & -A \\ -A & E_0 - \mu\varepsilon(t) \end{pmatrix}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}$$

or

$$\begin{aligned} i\hbar \frac{d}{dt}\begin{pmatrix} c_a(t) \\ c_s(t) \end{pmatrix} &= \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}^{-1} \begin{pmatrix} E_0 + \mu\varepsilon(t) & -A \\ -A & E_0 - \mu\varepsilon(t) \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix} \begin{pmatrix} c_a(t) \\ c_s(t) \end{pmatrix} \\ &= \begin{pmatrix} A + E_0 & \mu\varepsilon(t) \\ \mu\varepsilon(t) & -A + E_0 \end{pmatrix}\begin{pmatrix} c_a(t) \\ c_s(t) \end{pmatrix} \end{aligned}$$

First we write

$$c_a(t) = \gamma_a(t) e^{-\frac{i(E_0 + A)t}{\hbar}}$$

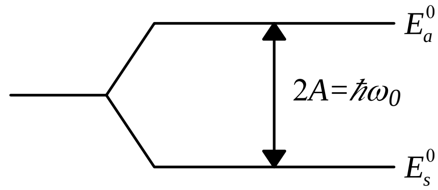
$$c_s(t) = \gamma_s(t) e^{-\frac{i(E_0 - A)t}{\hbar}}$$

$$i\hbar \frac{d\gamma_a(t)}{dt} = \mu\varepsilon(t) e^{i\omega_0 t}\gamma_s(t)$$

$$i\hbar \frac{d\gamma_s(t)}{dt} = \mu\varepsilon(t) e^{-i\omega_0 t}\gamma_a(t)$$

where

$$E_a^{(0)} - E_b^{(0)} = \hbar\omega_0 = 2A$$



We consider the case:

$$\varepsilon(t) = 2\varepsilon_0 \cos\omega t = \varepsilon_0 (e^{i\omega t} + e^{-i\omega t})$$

Then we have

$$i\hbar \frac{d\gamma_a(t)}{dt} = \mu\varepsilon_0 [e^{i(\omega+\omega_0)t} + e^{-i(\omega-\omega_0)t}]\gamma_s(t)$$

$$i\hbar \frac{d\gamma_s(t)}{dt} = \mu\varepsilon_0 [e^{i(\omega-\omega_0)t} + e^{-i(\omega+\omega_0)t}]\gamma_a(t)$$

29S.3 Rotating wave approximation

The terms with $(\omega + \omega_0)$ oscillate very rapidly about an average value of zero and, therefore do not contribute very much on the average to the rate of change of γ.

$$i \frac{d\gamma_a(t)}{dt} = \frac{\mu\varepsilon_0}{\hbar} e^{-i(\omega-\omega_0)t}\gamma_s(t) = \Gamma_0 e^{-i\Delta t}\gamma_s(t)$$

$$i \frac{d\gamma_s(t)}{dt} = \frac{\mu\varepsilon_0}{\hbar} e^{i(\omega-\omega_0)t}\gamma_a(t) = \Gamma_0 e^{i\Delta t}\gamma_a(t)$$

$$\gamma_a(0) = 1, \qquad \gamma_s(0) = 0$$

where

$$\Gamma_0 = \frac{\mu\varepsilon_0}{\hbar}, \qquad \Delta = \omega - \omega_0$$

$$\Omega = \sqrt{\frac{\Delta^2}{4} + \Gamma_0^{\,2}} \qquad \text{(Rabi frequency)}$$

Using the Mathematica (see below), we get the solution

$$\gamma_a(t) = \frac{e^{-\frac{1}{2}it(2\Omega+\Delta)}}{4\Omega}[2\Omega - \Delta + e^{i2\Omega t}(2\Omega + \Delta)]$$

$$\gamma_s(t) = -i\frac{\Gamma_0}{\Omega} e^{\frac{1}{2}it\Delta} \sin(\Omega t)\,.$$

The probability for finding the system in the antisymmetric state is

$$P_a = \frac{4\Omega^2 + \Delta^2 + (4\Omega^2 - \Delta^2)\cos(2\Omega t)}{8\Omega^2}$$
$$= \frac{2\Gamma_0{}^2 + \Delta^2 + 2\Gamma_0{}^2 \cos(\sqrt{\Delta^2 + 4\Gamma_0{}^2} t)}{\Delta^2 + 4\Gamma_0{}^2}$$

The probability for finding the system in the symmetric state is

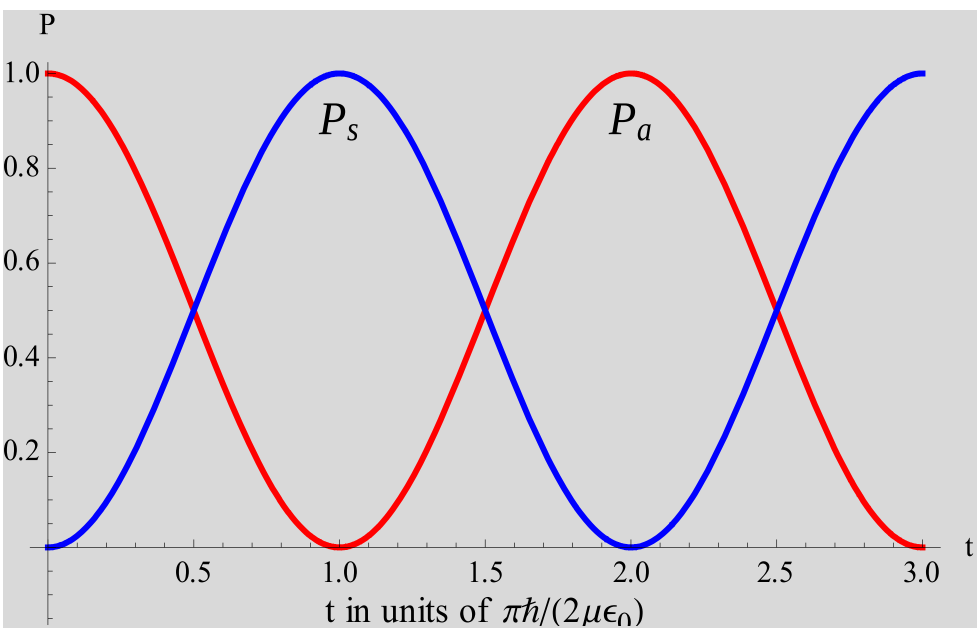
$$P_s = \frac{\Gamma_0{}^2 \sin^2(\Omega t)]}{\Omega^2}$$
$$= \frac{4\Gamma_0{}^2 \sin^2(\frac{1}{2}\sqrt{\Delta^2 + 4\Gamma_0{}^2} t)]}{\Delta^2 + 4\Gamma_0{}^2}$$

Note that

$$P_a + P_s = 1$$

When $\varDelta = 0$ (at resonance),

$$P_a = \cos^2(\Gamma_0 t), \qquad P_s = \sin^2(\Gamma_0 t).$$



Let us suppose that it takes the time T to go through the cavity. If we make the cavity just long enough so that $\mu\varepsilon_0 T/\hbar = \pi/2$, then a molecules which enters in the upper state $\left|\varphi_a^{(0)}\right\rangle$ will certainly leave it in the lower state $\left|\varphi_s^{(0)}\right\rangle$.

cavity

In other words, its energy is decreased, and the loss of energy cannot go anywhere else but into the machinery which generate the field.

In summary, the molecules enter the cavity, the cavity field-oscillating at exactly the right frequency-induces transition from the upper to the lower states, and the energy released is fed into the oscillatory field. The molecular energy is converted into the energy of an external electromagnetic field.

((**Mathematica**))

```
Clear["Global`*"];
```

$\Delta=\omega-\omega 0,\quad \sqrt{\Gamma 0^2+\frac{\Delta^2}{4}}=\Omega,\quad \Gamma 0=\frac{\mu\,\varepsilon 0}{\hbar}$

```
eq1 = ⅈ D[γa[t], t] == Γ0 Exp[-ⅈ Δ t] γs[t];

eq2 = ⅈ D[γs[t], t] == Γ0 Exp[ⅈ Δ t] γa[t];

s11 = DSolve[{eq1, eq2, γa[0] == 1, γs[0] == 0}, {γa[t], γs[t]}, t] //
  Simplify[#, {Δ > 0, Γ0 > 0}] &;
```

$$\texttt{s12 = s11 /. }\left\{\sqrt{4\,\Gamma 0^2+\Delta^2}\to 2\,\Omega,\ \frac{1}{\sqrt{4\,\Gamma 0^2+\Delta^2}}\to\frac{1}{2\,\Omega}\right\}\texttt{ // Simplify;}$$

```
γa[t_] = γa[t] /. s12[[1]] // FullSimplify
```

$$\frac{e^{-\frac{1}{2} i t (\Delta+2\Omega)}\left(-\Delta+2\Omega+e^{2 i t \Omega}(\Delta+2\Omega)\right)}{4\,\Omega}$$

```
γs[t_] = γs[t] /. s12[[1]] // FullSimplify
```

$$-\frac{i\, e^{\frac{i t \Delta}{2}}\,\Gamma 0\,\mathrm{Sin}[t\,\Omega]}{\Omega}$$

```
SuperStar /: expr_* := expr /. {Complex[a_, b_] :> Complex[a, -b]}

Pa = γa[t]* γa[t] // FullSimplify
```

$$\frac{\Delta^2+4\,\Omega^2-\left(\Delta^2-4\,\Omega^2\right)\mathrm{Cos}[2\,t\,\Omega]}{8\,\Omega^2}$$

$$\texttt{Pa1 = Pa /. }\left\{\Omega\to\frac{\sqrt{4\,\Gamma 0^2+\Delta^2}}{2}\right\}\texttt{ // Simplify}$$

$$\frac{2\,\Gamma 0^2+\Delta^2+2\,\Gamma 0^2\,\mathrm{Cos}\left[t\sqrt{4\,\Gamma 0^2+\Delta^2}\right]}{4\,\Gamma 0^2+\Delta^2}$$

```
Ps = γs[t]* γs[t] // FullSimplify
```

$$\frac{\Gamma 0^2\,\mathrm{Sin}[t\,\Omega]^2}{\Omega^2}$$

$$\texttt{Ps1 = Ps /. }\left\{\Omega\to\frac{\sqrt{4\,\Gamma 0^2+\Delta^2}}{2}\right\}\texttt{ // Simplify}$$

$$\frac{4\,\Gamma 0^2\,\mathrm{Sin}\left[\frac{1}{2}\,t\sqrt{4\,\Gamma 0^2+\Delta^2}\right]^2}{4\,\Gamma 0^2+\Delta^2}$$

```
Pa1 + Ps1 // Simplify
```

1

```
Pa2 = Pa1 /. Δ → 0 // Simplify[#, Γ0 > 0] &
```

$\mathrm{Cos}[t\,\Gamma 0]^2$

```
Ps2 = Ps1 /. Δ → 0 // Simplify[#, Γ0 > 0] &
```

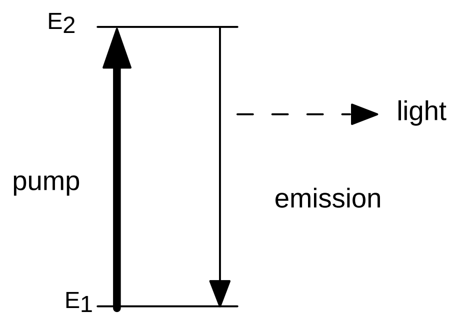
$\mathrm{Sin}[t\,\Gamma 0]^2$

29S.4 Laser Physics

Light amplification by stimulated emission of radiation. A laser operates by adsorbing energy and emitting it at a well-defined wavelength by a stimulated emission process (Einstein *A*, *B* coefficient).

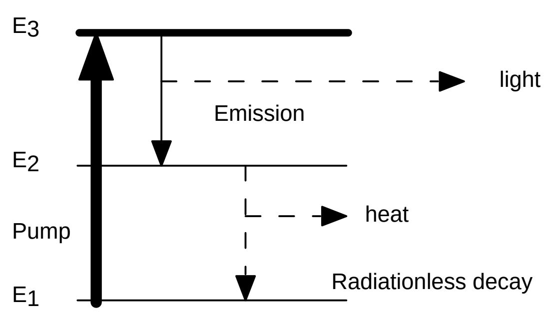
A two-level laser

It is necessary to remove more than 50 % of the atoms from their ground state into the excited state.



A three-level laser

The population-inversion is much easier to attain, especially if the lower excited state can relax rapidly into the ground state.



We consider the two level-system in the Dirac picture

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

with

$$\left|\psi_I(t)\right\rangle = e^{\frac{i\hat{H}_0 t}{\hbar}}\left|\psi_S(t)\right\rangle$$

$$i\hbar\frac{\partial}{\partial t}\left\langle n\middle|\psi_I(t)\right\rangle = \sum_m \left\langle n\middle|\hat{V}_I(t)\middle|m\right\rangle\left\langle m\middle|\psi_I(t)\right\rangle$$

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

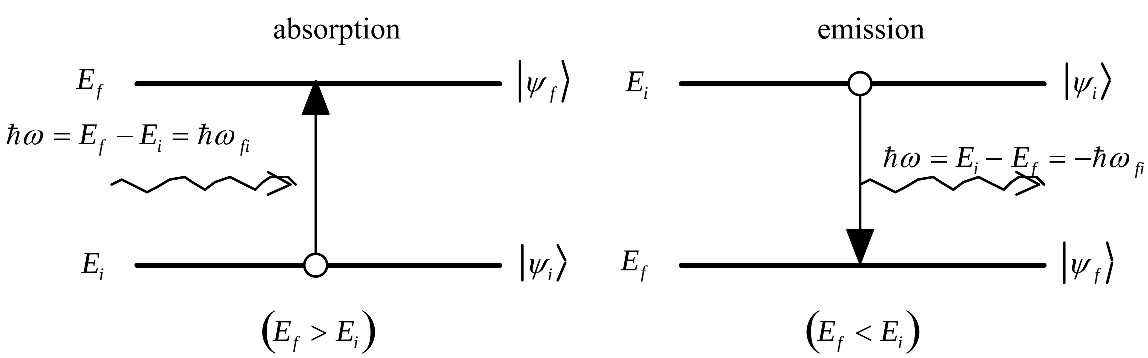
$$\left\langle n\middle|\hat{V}_I(t)\middle|m\right\rangle = e^{\frac{i}{\hbar}(E_n - E_m)t}\left\langle n\middle|\hat{V}_s(t)\middle|m\right\rangle = e^{i\omega_{nm}t}\left\langle n\middle|\hat{V}_s(t)\middle|m\right\rangle$$

where

$$\hat{V}_s(t) = \hat{V}e^{i\omega t} + \hat{V}^{+}e^{-i\omega t}$$

$$\hbar\omega_{nm} = (E_n - E_m), \qquad \text{Bohr frequency}$$

$$i\hbar\frac{\partial}{\partial t}c_n(t) = \sum_m e^{i\omega_{nm}t}\left\langle n\middle|\hat{V}_s(t)\middle|m\right\rangle c_m(t)$$



n = 1 and 2 (two-level system)

$$i\hbar\begin{pmatrix}\dot{c}_1\\ \dot{c}_2\end{pmatrix} = \begin{pmatrix}\left\langle 1\middle|\hat{V}_s(t)\middle|1\right\rangle & \left\langle 1\middle|\hat{V}_s(t)\middle|2\right\rangle e^{i\omega_{12}t}\\ \left\langle 2\middle|\hat{V}_s(t)\middle|1\right\rangle e^{-i\omega_{21}t} & \left\langle 2\middle|\hat{V}_s(t)\middle|2\right\rangle\end{pmatrix}\begin{pmatrix}c_1\\ c_2\end{pmatrix}$$

$$\begin{aligned}\left\langle 1\middle|\hat{V}_s(t)\middle|2\right\rangle e^{i\omega_{12}} &= \left\langle 1\middle|\hat{V}e^{i\omega t} + \hat{V}^{+}e^{-i\omega t}\middle|2\right\rangle e^{i\omega_{12}t}\\ &= \left\langle 1\middle|\hat{V}\middle|1\right\rangle e^{i(\omega_{12}t + \omega t)} + \left\langle 1\middle|\hat{V}^{+}\middle|2\right\rangle e^{-i(\omega - \omega_{12})t}\end{aligned}$$

$$\langle 2|\hat{V}_s(t)|1\rangle e^{-i\omega_{12}t} = \langle 2|\hat{V}e^{i\omega t} + \hat{V}^+ e^{-i\omega t}|1\rangle e^{-i\omega_{12}t}$$
$$= \langle 2|\hat{V}|1\rangle e^{i(-\omega_{12}t+\omega t)} + \langle 2|\hat{V}^+|1\rangle e^{-i(\omega+\omega_{12})t}$$

We assume that

$$\langle 1|\hat{V}_s(t)|1\rangle = 0$$

$$\langle 2|\hat{V}_s(t)|2\rangle = 0$$

$$\langle 1|\hat{V}_s(t)|2\rangle e^{i\omega_{12}} \approx \langle 1|\hat{V}|2\rangle e^{i(-\omega_{21}t+\omega t)} = \gamma e^{i\Delta t}$$

$$\langle 2|\hat{V}_s(t)|1\rangle e^{-i\omega_{12}t} = \langle 2|\hat{V}^+|1\rangle e^{-i(\omega-\omega_{21})t} = \gamma e^{-i\Delta t}$$

where

$$\Delta = \omega - \omega_{21}, \qquad \gamma = \langle 1|\hat{V}|2\rangle .$$

Then we have

$$i\hbar\frac{\partial}{\partial t}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 0 & \gamma e^{i\Delta t} \\ \gamma e^{-i\Delta\omega t} & 0 \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

Initial condition:

$$c_1(0) = 1, \qquad c_2(0) = 0$$

$$i\dot{c}_1(t) = \frac{\gamma}{\hbar}e^{i\Delta t}c_2(t) = \Gamma_0 e^{i\Delta t}c_2(t) \tag{1}$$

$$i\dot{c}_2(t) = \frac{\gamma}{\hbar}e^{-i\Delta t}c_1(t) = \Gamma_0 e^{-i\Delta t}c_1(t) \tag{2}$$

where

$$\Gamma_0 = \frac{\gamma}{\hbar}$$

and

$$\Omega = \sqrt{\frac{\Delta^2}{4} + {\Gamma_0}^2}\,, \qquad\qquad \text{(Rabi frequency).}$$

The solutions for $c_1(t)$ and $c_2(t)$ are given by

$$c_1(t) = \frac{e^{-\frac{1}{2}it(2\Omega-\Delta)}}{4\Omega}[2\Omega + \Delta + e^{i2\Omega t}(2\Omega - \Delta)]$$

and

$$c_2(t) = -i\frac{\Gamma_0}{\Omega}e^{-\frac{1}{2}it\Delta}\sin(\Omega t)$$

respectively.

The probability that at a time t the system is in the lower state is

$$P_1(t) = \left|C_1(t)\right|^2 = 1 - \frac{4{\Gamma_0}^2}{4{\Gamma_0}^2 + \Delta^2}\sin^2(\frac{t}{2}\sqrt{4{\Gamma_0}^2 + \Delta^2})$$

The probability that a time t the system is in the upper state is

$$P_2(t) = \left|C_2(t)\right|^2 = \frac{4{\Gamma_0}^2}{4{\Gamma_0}^2 + \Delta^2}\sin^2(\frac{t}{2}\sqrt{4{\Gamma_0}^2 + \Delta^2})$$

With the perfect tuning ($\Delta = 0$),

$$P_2(t) = \sin^2(\Gamma_0 t)\,, \qquad \text{and} \qquad P_1(t) = \cos^2(\Gamma_0 t)$$

The system returns to its original state after a time $T = 2\pi/\Gamma_0$.

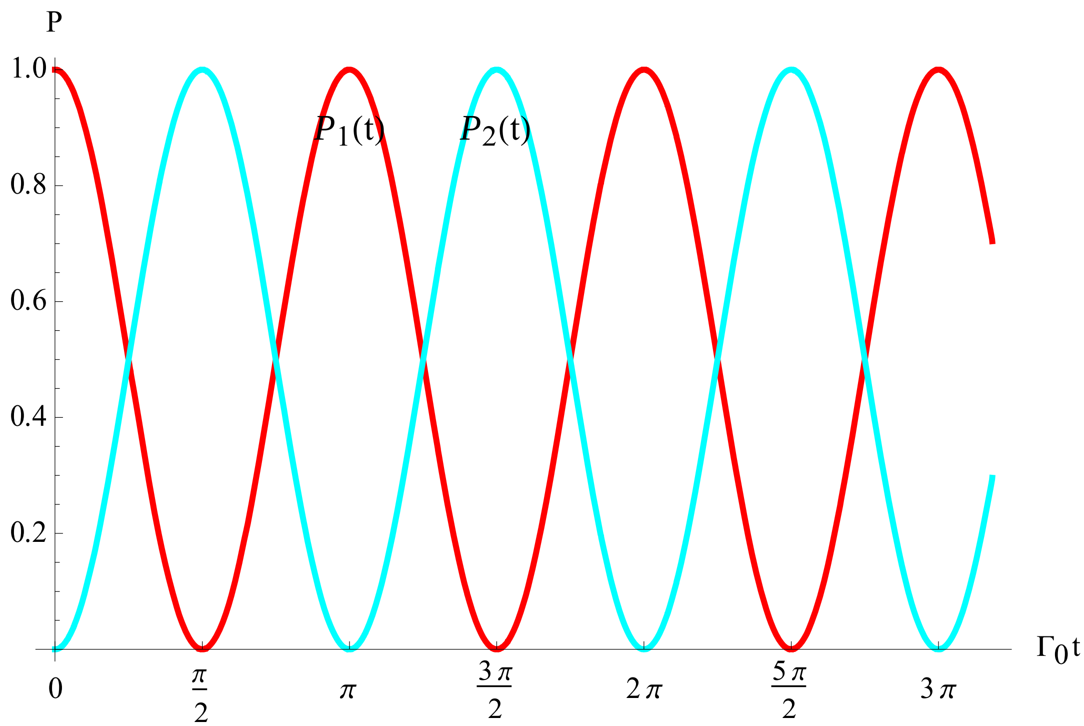


Fig. Time dependence of $P_1(t)$ (red) and $P_2(t)$ (blue), The parameter $\Delta = \omega - \omega_{12} = 0$. $P_1(t) + P_2(t) = 1$. The absorption occurs for $\Gamma_0\, t = n\,\pi - (n+1/2)\pi$ (n = 0, 1, 2, ...), while the absorption occurs for $\Gamma_0\, t = (n+1/2)\pi - n\pi$ (n = 0, 1, 2, ...).

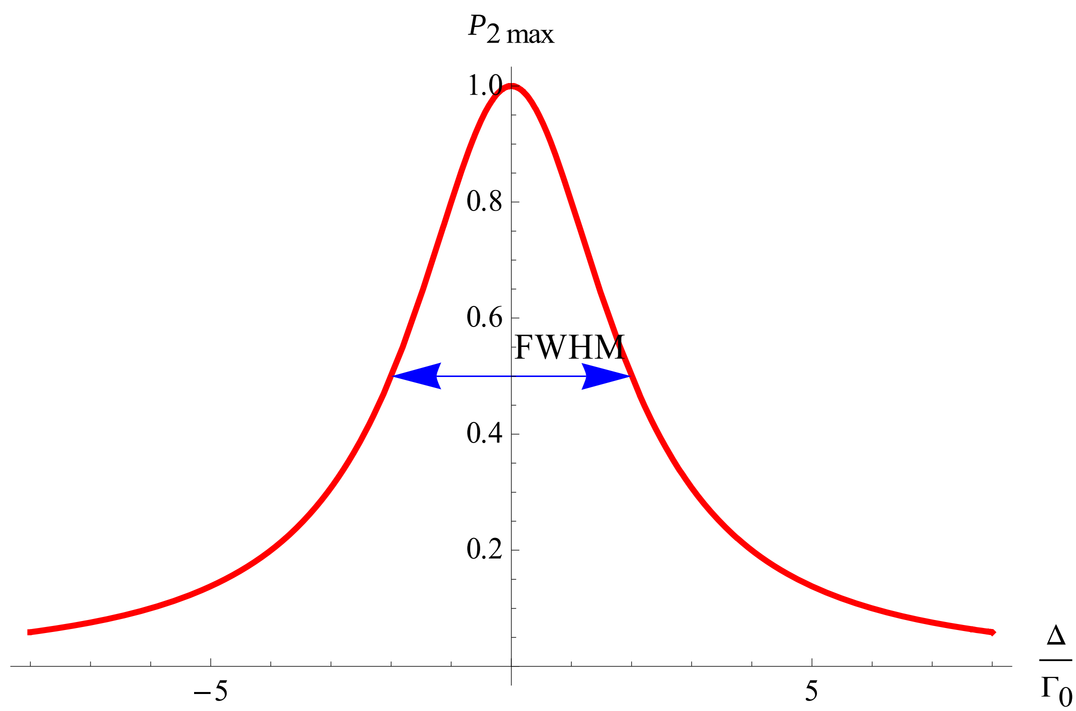


Fig. Plot of the maximum of the probability P_2 as a function of Δ/Γ_0. FWHM (full-width at half maximum) $4\Gamma_0$.

29S.5 Induced electric dipole moment

$$\hat{V}_s(t) = \hat{V}e^{i\omega t} + \hat{V}^{+}e^{-i\omega t}$$

where

$$\hat{V} = -q\hat{z}\varepsilon_0$$

with $q<0$ and ε_0 is the amplitude of electric field.

$$\gamma = \langle 1|\hat{V}|2\rangle = \langle 1|-q\hat{z}\varepsilon_0|2\rangle = -q\varepsilon_0\langle 1|\hat{z}|2\rangle$$

or

$$\langle 1|\hat{z}|2\rangle = -\frac{\gamma}{q\varepsilon_0}$$

We calculate the expectation of the electric dipole moment $p(t)$

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

$$|\psi_I(t)\rangle = \begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}, \qquad \langle\psi_I(t)| = \begin{pmatrix} c_1^*(t) & c_2^*(t) \end{pmatrix}$$

$$e^{\frac{i}{\hbar}\hat{H}_0 t}(-q\varepsilon_0\hat{z})e^{-\frac{i}{\hbar}\hat{H}_0 t} = \begin{pmatrix} e^{\frac{i}{\hbar}E_1 t} & 0 \\ 0 & e^{\frac{i}{\hbar}E_2 t} \end{pmatrix}\begin{pmatrix} 0 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & 0 \end{pmatrix}\begin{pmatrix} e^{-\frac{i}{\hbar}E_1 t} & 0 \\ 0 & e^{-\frac{i}{\hbar}E_2 t} \end{pmatrix}$$
$$= \begin{pmatrix} 0 & \gamma e^{i\Delta t} \\ \gamma e^{-i\Delta t} & 0 \end{pmatrix}$$

or

$$e^{\frac{i}{\hbar}\hat{H}_0 t}(q\hat{z})e^{-\frac{i}{\hbar}\hat{H}_0 t} = -\frac{1}{\varepsilon_0}\begin{pmatrix} 0 & \gamma e^{i\Delta t} \\ \gamma e^{-i\Delta t} & 0 \end{pmatrix}$$

Then the electric dipole moment $p(t)$ is given by

$$p(t) = (-\frac{1}{\varepsilon_0})\begin{pmatrix} c_1^*(t) & c_2^*(t) \end{pmatrix}\begin{pmatrix} 0 & \gamma e^{i\Delta t} \\ \gamma e^{-i\Delta t} & 0 \end{pmatrix}\begin{pmatrix} c_1(t) \\ c_2(t) \end{pmatrix}$$

$$\begin{aligned} p(t) &= (-\frac{\gamma}{\varepsilon_0})[e^{i\Delta t}c_1^*(t)c_2(t) + e^{-i\Delta t}c_1(t)c_2^*(t)] \\ &= -\frac{\hbar\Gamma_0^{\ 2}\Delta}{\varepsilon_0\Omega^2}\sin^2(\Omega t) \\ &= -\frac{\hbar\Gamma_0}{\varepsilon_0}\frac{4\Delta\Gamma_0}{\Delta^2 + 4\Gamma_0^{\ 2}}\sin^2(\sqrt{\frac{\Delta^2}{4} + \Gamma_0^{\ 2}}t) \end{aligned}$$

where

$$\Delta = \omega - \omega_{21}, \qquad \Omega = \sqrt{\frac{\Delta^2}{4} + \Gamma_0^{\ 2}}$$

and

$$\omega_{21} = \frac{1}{\hbar}(E_2 - E_1)$$

29S.6 Nuclear magnetic resonance: formulation

Proton has a magnetic moment 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 (=2.0) is the nuclear g factor, and μ_p is the magnetic moment; μ_p = 2.79270 μ_N = 1.410606633 x10^{-23} emu. γ is the gyromagnetic ratio, given by

$$\gamma = \frac{g_N\mu_p}{\hbar}$$

and μ_N is the nuclear magneton: $\mu_N = \dfrac{e\hbar}{2M_pc}$=5.05951 x 10^{-24} emu.

We consider the magnetic moment

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

in the presence of magnetic fields, $\boldsymbol{B} = B_0\, \boldsymbol{e}_z$.The Hamiltonian is given by

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

The eigenstate:

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

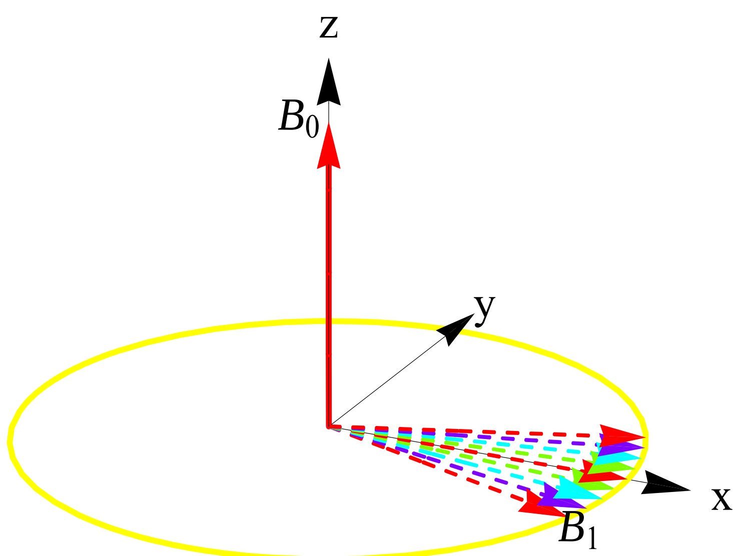
$$E_- - E_+ = \gamma\hbar B_0 = \hbar\omega_0$$

where

$$f_o \text{ (MHz)} = \omega_0/2\pi = 4.258 \text{ B}_0 \text{ (kOe)}$$

Further we apply the AC magnetic field $\boldsymbol{B}_1 = 2\, B_1 \cos(\omega t)\, \boldsymbol{e}_x$ (lineary polarized) is given by

$$\begin{aligned}\mathbf{B}_1 &= 2B_1 \cos(\omega t)\mathbf{e}_x \\ &= [B_1 \cos(\omega t)\mathbf{e}_x + B_1 \sin(\omega t)\mathbf{e}_y] + [B_1 \cos(\omega t)\mathbf{e}_x - B_1 \sin(\omega t)\mathbf{e}_y]\end{aligned}$$



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

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

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

$$\begin{aligned}\hat{H} &= -\mu \cdot \mathbf{B}(t) \\ &= -\gamma \frac{\hbar}{2}(\mathbf{B} \cdot \boldsymbol{\sigma}) \\ &= -\gamma \frac{\hbar}{2}[B\sigma_z + B_1 \cos(\omega t)\sigma_x - B_1 \cos(\omega t)\sigma_y]\end{aligned}$$

or

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

Suppose that the eigenket is given by

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

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

Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = i\hbar \begin{pmatrix} \frac{da_1}{dt} \\ \frac{da_2}{dt} \end{pmatrix}$$

$$= \hat{H}\begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix} = -\gamma \frac{\hbar}{2}\begin{pmatrix} B_0 & B_1 e^{i\omega t} \\ -B_1 e^{i\omega t} & B_0 \end{pmatrix}\begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix}$$

or

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

Unitary transformation:

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

$$|\psi'(t)\rangle = \hat{U}(t)|\psi(t)\rangle = \begin{pmatrix} b_1(t) \\ b_2(t) \end{pmatrix} = \begin{pmatrix} e^{-\frac{i}{2}\omega t} & 0 \\ 0 & e^{\frac{i}{2}\omega t} \end{pmatrix}\begin{pmatrix} a_1(t) \\ a_2(t) \end{pmatrix}$$

or

$$a_1(t) = \exp(\frac{i}{2}\omega t) b_1(t)$$

$$a_2(t) = \exp(-\frac{i}{2}\omega t) b_2(t)$$

Then we have

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

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

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

Thus

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

For simplicity we put

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

We now consider the Schrödinger equation,

$$i\hbar\begin{pmatrix} \frac{db_1}{dt} \\ \frac{db_2}{dt} \end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix} \Delta & -\omega_1 \\ -\omega_1 & -\Delta \end{pmatrix}\begin{pmatrix} b_1 \\ b_2 \end{pmatrix}$$

or

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

where

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

and

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

The solution of this equation is given by

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

29S.7 Eigenvalue problem

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

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

or

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

or

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

where

$$(\hat{\sigma}\cdot\mathbf{n})\left|\pm\right\rangle_n = \pm\left|\pm\right\rangle_n$$

or

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

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

$$E = \hbar\Omega$$

with

$$\Omega = \frac{1}{2}\sqrt{\Delta^2+\omega_1^2}$$

$$\left|+\right\rangle_n = \cos(\frac{\theta}{2})\left|+\right\rangle + \sin(\frac{\theta}{2})\left|-\right\rangle$$

$$\left|+\right\rangle_n = -\sin(\frac{\theta}{2})\left|+\right\rangle + \cos(\frac{\theta}{2})\left|-\right\rangle$$

where

$$\cos\theta = \frac{-\Delta}{\sqrt{\Delta^2+\omega_1^2}} = \frac{-2\Delta}{\Omega},$$

$$\sin\theta = \frac{\omega_1}{\sqrt{\Delta^2+\omega_1^2}} = \frac{2\Delta}{\Omega}$$

Here

$$\left|+\right\rangle = \cos(\frac{\theta}{2})\left|+\right\rangle_n - \sin(\frac{\theta}{2})\left|-\right\rangle_n$$

29S.8 Transition probability: Rabi's formula

We assume that the initial condition is given by

$$\left|\psi'(t=0)\right\rangle = \left|\psi(t=0)\right\rangle = \left|+\right\rangle$$

What is the probability $P_{+-}(t)$ for finding the spin in the state $\left|-\right\rangle$

$$\left|\psi'(t)\right\rangle = \exp(-\frac{i\hat{H}'t}{\hbar})\left|+\right\rangle = \exp(-\frac{i\hat{H}'t}{\hbar})[\cos(\frac{\theta}{2})\left|+\right\rangle_n - \sin(\frac{\theta}{2})\left|-\right\rangle_n]$$
$$= \exp(i\Omega t)[\cos(\frac{\theta}{2})\left|+\right\rangle_n - \sin(\frac{\theta}{2})\exp(-i\Omega t)\left|-\right\rangle_n]$$

or

$$\left\langle - \middle| \psi'(t)\right\rangle = \exp(i\Omega t)[\cos(\frac{\theta}{2})\left\langle - \middle| + \right\rangle_n - \sin(\frac{\theta}{2})\exp(-i\Omega t)\left\langle - \middle| + \right\rangle_n]$$
$$= \cos(\frac{\theta}{2})\sin(\frac{\theta}{2})[\exp(i\Omega t) - \exp(-i\Omega t)]$$
$$= i\sin\theta\sin(\Omega t)$$
$$= i\frac{\omega_1}{2\Omega}\sin(\Omega t)$$

Then the Rabi's formula becomes

$$P_{+-}(t)=\frac{\omega_1{}^2}{4\Omega^2}\sin^2(\Omega t)=\frac{\omega_1{}^2}{\Delta^2+\omega_1^2}\sin^2\left(\frac{t}{2}\sqrt{\Delta^2+\omega_1^2}\right)$$

((Mathematica))

We calculate the matrix $\exp(-\frac{i\hat{H}'}{\hbar}t)$ directly using Mathematica.

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

Claculation of $\exp\left(\frac{-i}{\hbar}\text{H1 t}\right)$

```
Clear["Global`*"];

σz = (1  0
      0 -1); σx = (0 1
                   1 0);

H1 = ℏ/2 (Δ σz - ω1 σx);

s1 = MatrixExp[-ⅈ/ℏ H1 t] // Simplify;

rule1 = {Sqrt[-Δ^2 - ω1^2] → ⅈ 2 Ω, 1/Sqrt[-Δ^2 - ω1^2] → 1/(ⅈ 2 Ω)};

s11 = s1 /. rule1 // FullSimplify;
s11 // MatrixForm
```

$$\begin{pmatrix}\text{Cos}[t\,\Omega]-\frac{i\,\Delta\,\text{Sin}[t\,\Omega]}{2\,\Omega} & \frac{i\,\omega1\,\text{Sin}[t\,\Omega]}{2\,\Omega}\\ \frac{i\,\omega1\,\text{Sin}[t\,\Omega]}{2\,\Omega} & \text{Cos}[t\,\Omega]+\frac{i\,\Delta\,\text{Sin}[t\,\Omega]}{2\,\Omega}\end{pmatrix}$$

```
s11 // MatrixForm
```

$$\begin{pmatrix}\text{Cos}[t\,\Omega]-\frac{i\,\Delta\,\text{Sin}[t\,\Omega]}{2\,\Omega} & \frac{i\,\omega1\,\text{Sin}[t\,\Omega]}{2\,\Omega}\\ \frac{i\,\omega1\,\text{Sin}[t\,\Omega]}{2\,\Omega} & \text{Cos}[t\,\Omega]+\frac{i\,\Delta\,\text{Sin}[t\,\Omega]}{2\,\Omega}\end{pmatrix}$$

$$\Omega=\frac{1}{2}\sqrt{\Delta^2+\omega_1^2}$$

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

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

where

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

We assume that

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

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

$$P_{+-} = \left|b_2\right|^2 = \frac{\omega_1^2\sin^2(\Omega t)}{4\Omega^2}$$

$$P_{++} = \left|b_1\right|^2 = 1 - \frac{\omega_1^2\sin^2(\Omega t)}{4\Omega^2}$$

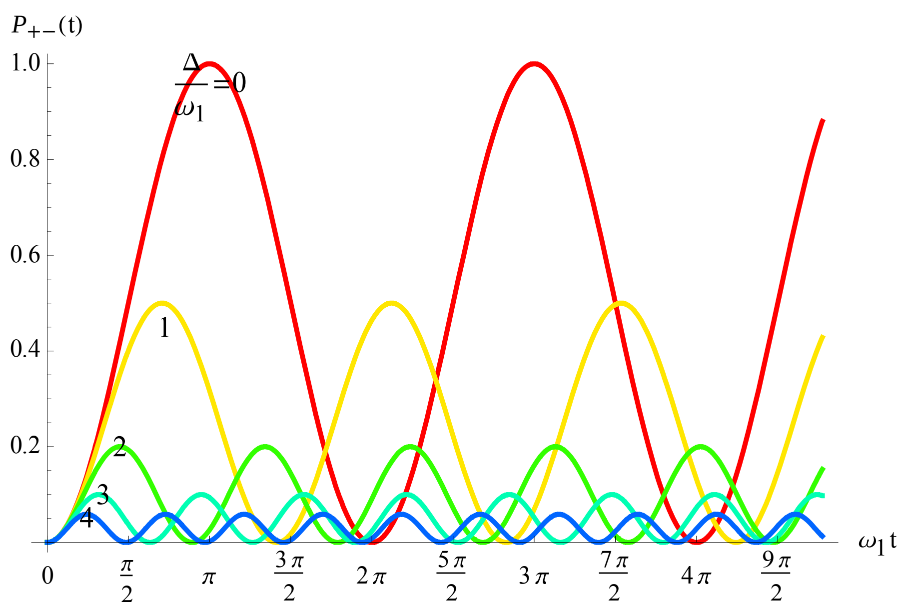


Fig. Plot of $P_{+-}(t)$ vs $\omega_1 t$, where Δ/ω_1 is changed as a parameter. $\Delta = \omega - \omega_1$.

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