Hamiltonianos que variam no tempo

Hamiltonianos dependente do tempo...   (*bye-bye* autoestados estacionários!!)
Probabilidade de transição, Oscilações de Rabi...

Hamiltonianos dependentes do tempo

Deseja-se resolver:

$$\boxed{\hat{H} = \hat{H}_o + \hat{V}(t)}$$

$$\boxed{i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle}$$

Suponha que conhecemos

$$\hat{H}_o\,|\psi_n\rangle = E_n\,|\psi_n\rangle$$

$$\langle\psi_m|\psi_n\rangle = \delta_{mn}$$

Expansão na base dos estados estacionários de $\hat{H}_o$...

$$|\Psi\rangle = \sum_n c_n(t)\exp\left(-iE_nt/\hbar\right)|\psi_n\rangle$$

Postulado 6: evolução dinâmica do sistema

Aula 1

Schrödinger Picture

A evolução temporal do vetor de estado de um sistema quântico fechado é dada pela equação de Schrödinger.

$$i\hbar \frac{\partial}{\partial t} |\psi_s(t)\rangle = \hat{H} |\psi_s(t)\rangle$$

$e^{-iE_3t/\hbar}$

Para Hamiltoniano independente do tempo, temos:

$$|\psi_s(t)\rangle = \exp\left(-\frac{i}{\hbar}\hat{H}(t-t_o)\right)|\psi_s(t_o)\rangle$$

A exponencial define o ***operador unitário de evolução temporal***

$$\hat{U}(t,t_o) = \exp\left(-\frac{i}{\hbar}\hat{H}(t-t_o)\right)$$

que evolui o vetor de estado $|\psi(t_o)\rangle \to |\psi(t)\rangle$, tal que:

$$|\psi_s(t)\rangle = \hat{U}(t,t_o)\,|\psi_s(t_o)\rangle \,.$$

Evolução temporal é no ***vetor de estado***

Postulado 6: evolução dinâmica do sistema

Aula 1

Interaction Picture

Representação particularmente útil em problemas onde o Hamiltoniano depende explicitamente do tempo e pode ser dividido em duas partes:

$V(t)$

$$\hat{H}(t) = \hat{H}_0 + \hat{H}_1(t)$$

Neste caso, temos

$$|\psi_I(t)\rangle = \exp\left(i\hat{H}_o(t-t_o)/\hbar\right)|\psi_S(t)\rangle$$

$$\hat{A}_I(t) = \exp\left(i\hat{H}_o(t-t_o)/\hbar\right)\cdot\hat{A}_S\cdot\exp\left(-i\hat{H}_o(t-t_o)/\hbar\right)$$

Definindo $\hat{H}_I = \exp\left(i\hat{H}_o(t-t_o)/\hbar\right)\cdot\hat{H}_1\cdot\exp\left(-i\hat{H}_o(t-t_o)/\hbar\right)$

Temos $i\hbar\frac{\partial}{\partial t}|\psi_I(t)\rangle = \hat{H}_I|\psi_I(t)\rangle$ e $\frac{d}{dt}\hat{A}_I = \frac{1}{i\hbar}[\hat{A}_I, \hat{H}_I] + \frac{\partial \hat{A}_I}{\partial t}$

Evolução temporal tanto do ***vetor de estado*** como do ***operador***

Hamiltonianos dependentes do tempo

Deseja-se resolver:

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

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle$$

Suponha que conhecemos

$$\hat{H}_o\,|\psi_n\rangle = E_n\,|\psi_n\rangle$$

$$\langle\psi_m|\psi_n\rangle = \delta_{mn}$$

$$|\Psi\rangle = \sum_n \underbrace{c_n(t)\exp\left(-iE_n t/\hbar\right)}\,|\psi_n\rangle \Rightarrow \boxed{|\Psi(t)\rangle}$$

Hamiltonianos dependentes do tempo

Deseja-se resolver: $|\Psi(t)\rangle$

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

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle$$

$$|\Psi\rangle = \sum_n c_n(t)\exp\left(-iE_n t/\hbar\right)|\psi_n\rangle$$

Suponha que conhecemos

$$\hat{H}_o\,|\psi_n\rangle = E_n\,|\psi_n\rangle$$

$$\langle\psi_m|\psi_n\rangle = \delta_{mn}$$

$$\sum_n \left(i\hbar\,\dot{c}_n + c_n E_n\right)\exp\left(-iE_n t/\hbar\right)|\psi_n\rangle = \sum_n c_n\left(\hat{H}_o + \hat{V}(t)\right)\exp\left(-iE_n t/\hbar\right)|\psi_n\rangle$$

$$\dot{c}_n \equiv \frac{\partial c_n}{\partial t} = \frac{d\,c_n}{dt}$$

Hamiltonianos dependentes do tempo

Deseja-se resolver: $|\Psi(t)\rangle$

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

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle$$

Suponha que conhecemos

$$\hat{H}_o\,|\psi_n\rangle = E_n\,|\psi_n\rangle$$

$$\langle\psi_m|\psi_n\rangle = \delta_{mn}$$

$$|\Psi\rangle = \sum_n c_n(t)\exp\left(-iE_nt/\hbar\right)|\psi_n\rangle$$

$$\langle\psi_m|\left[\sum_n \left(i\hbar\,\dot{c}_n + c_nE_n\right)\exp\left(-iE_nt/\hbar\right)|\psi_n\rangle = \sum_n c_n\left(\hat{H}_o + \hat{V}(t)\right)\exp\left(-iE_nt/\hbar\right)|\psi_n\rangle\right]$$

$$\dot{c}_n \equiv \frac{\partial\,c_n}{\partial t} = \frac{d\,c_n}{dt}$$

$$i\hbar\,\dot{c}_m(t)\exp\left(-iE_mt/\hbar\right) =$$

$$= \sum_n c_n(t)\exp\left(-iE_nt/\hbar\right)\left\langle\psi_m\left|\hat{V}(t)\right|\psi_n\right\rangle$$

Hamiltonianos dependentes do tempo

Deseja-se resolver:

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

$$i\hbar\frac{\partial}{\partial t}|\Psi\rangle = \hat{H}|\Psi\rangle$$

$$|\Psi\rangle = \sum_n c_n(t)\exp\left(-iE_n t/\hbar\right)|\psi_n\rangle$$

$$i\hbar\ \dot{c}_m(t)\exp\left(-iE_m t/\hbar\right) = \sum_n c_n(t)\exp\left(-iE_n t/\hbar\right)\left\langle \psi_m \left| \hat{V}(t) \right| \psi_n \right\rangle$$

Hamiltonianos dependentes do tempo

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$$i\hbar\, \dot{c}_m(t) \exp\left(-iE_m t/\hbar\right) = \sum_n c_n(t) \exp\left(-iE_n t/\hbar\right)\left\langle \psi_m \left| \hat{V}(t) \right| \psi_n \right\rangle$$

$$\boxed{i\hbar\, \dot{c}_m(t) = \sum_n V_{mn} e^{i\omega_{mn} t} c_n(t)}$$

$$\boxed{\omega_{mn} \equiv \frac{(E_m - E_n)}{\hbar}}$$

$$i\hbar \begin{pmatrix} \dot{c}_1 \\ \dot{c}_2 \\ \dot{c}_3 \\ \vdots \end{pmatrix} = \begin{pmatrix} V_{11} & V_{12}e^{i\omega_{12}t} & & \cdots \\ V_{21}e^{i\omega_{21}t} & V_{22} & & \cdots \\ & & V_{33} & \cdots \\ \vdots & \vdots & & \ddots \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ c_3 \\ \vdots \end{pmatrix}$$

Até aqui, a resolução é exata...

Exemplo: *sistema dois níveis*

$E_2 > E_1$

Deseja-se resolver:

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

$$i\hbar\, \dot{c}_m(t) = \sum_n V_{mn} e^{i\omega_{mn} t} c_n(t)$$

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

Exemplo: *sistema dois níveis + potencial harmônico*

$e^{i\omega t} = \cos(\omega t) + i\,\mathrm{sen}(\omega t)$

Deseja-se resolver:

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

$$i\hbar\, \dot{c}_m(t) = \sum_n V_{mn} e^{i\omega_{mn}t} c_n(t)$$

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

$$i\hbar \begin{pmatrix} \dot{c}_1 \\ \dot{c}_2 \end{pmatrix} = \begin{pmatrix} 0 & \gamma e^{i(\omega_{12}+\omega)t} \\ \gamma e^{i(\omega_{21}-\omega)t} & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$\hat{H}_o = E_1 |1\rangle\langle 1| + E_2 |2\rangle\langle 2|\,; \quad (E_2 > E_1)$$

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

$$H = \begin{pmatrix} E_1 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & E_2 \end{pmatrix}$$

$$i\hbar\begin{pmatrix}\dot{c}_1\\ \dot{c}_2\end{pmatrix}=\begin{pmatrix}V_{11} & V_{12}e^{i\omega_{12}t}\\ V_{21}e^{i\omega_{21}t} & V_{22}\end{pmatrix}\begin{pmatrix}c_1\\ c_2\end{pmatrix}=\begin{pmatrix}0 & \gamma e^{i(\omega_{12}+\omega)t}\\ \gamma e^{i(\omega_{21}-\omega)t} & 0\end{pmatrix}\begin{pmatrix}c_1\\ c_2\end{pmatrix}$$

$$\left\{\begin{aligned}\dot{c}_1&=\frac{1}{i\hbar}\gamma e^{i(\omega_{12}-\omega)t}\cdot c_2\\ \dot{c}_2&=\frac{1}{i\hbar}\gamma e^{i(\omega_{21}-\omega)t}\cdot c_1\end{aligned}\right.$$

$$\boxed{\begin{aligned}c_1(0)&=1\\ c_2(0)&=0\end{aligned}}\Rightarrow c_2(t)=\frac{\gamma}{i\hbar}\int_0^t e^{i(\omega_{21}-\omega)t'}dt'=\frac{\gamma}{i\hbar}\left[\frac{e^{i(\omega_{21}-\omega)t}-1}{i(\omega_{21}-\omega)}\right]$$

$$c_2(t)=-\frac{\gamma}{\hbar}\frac{e^{i(\omega_{21}-\omega)t/2}}{(\omega_{21}-\omega)}\Big[\underbrace{e^{i(\omega_{21}-\omega)t/2}-e^{-i(\omega_{21}-\omega)t/2}}_{(2i)\cdot\,\mathrm{Sen}[(\omega_{21}-\omega)t/2]}\Big]$$

$$c_2(t)=-2i\frac{\gamma}{\hbar}\frac{e^{i(\omega_{21}-\omega)t/2}}{(\omega_{21}-\omega)}\cdot\mathrm{Sen}\left[(\omega_{21}-\omega)t/2\right]\Longrightarrow\boxed{\begin{array}{c}\text{Probabilidades}\\ |c_2(t)|^2\end{array}}$$

Exemplo: *sistema dois níveis + potencial harmônico*

Deseja-se resolver:

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

$$i\hbar\, \dot{c}_m(t) = \sum_n V_{mn} e^{i\omega_{mn}t} c_n(t)$$

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$$\hat{H}_o = E_1|1\rangle\langle 1| + E_2|2\rangle\langle 2|\,; \quad (E_2 > E_1)$$

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

$$H = \begin{pmatrix} E_1 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & E_2 \end{pmatrix}$$

Fórmula de Rabi

$$|c_2(t)|^2 = \frac{\gamma^2/\hbar^2}{\gamma^2/\hbar^2 + (\omega - \omega_{21})^2/4} \sin^2\left\{ \left[\frac{\gamma^2}{\hbar^2} + \frac{(\omega-\omega_{21})^2}{4} \right]^{1/2} t \right\}$$

$$|c_1(t)|^2 = 1 - |c_2(t)|^2$$

Exemplo: *sistema dois níveis* (osc. de Rabi)

Deseja-se resolver:

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

$$i\hbar\,\dot{c}_m(t) = \sum_n V_{mn} e^{i\omega_{mn}t} c_n(t)$$

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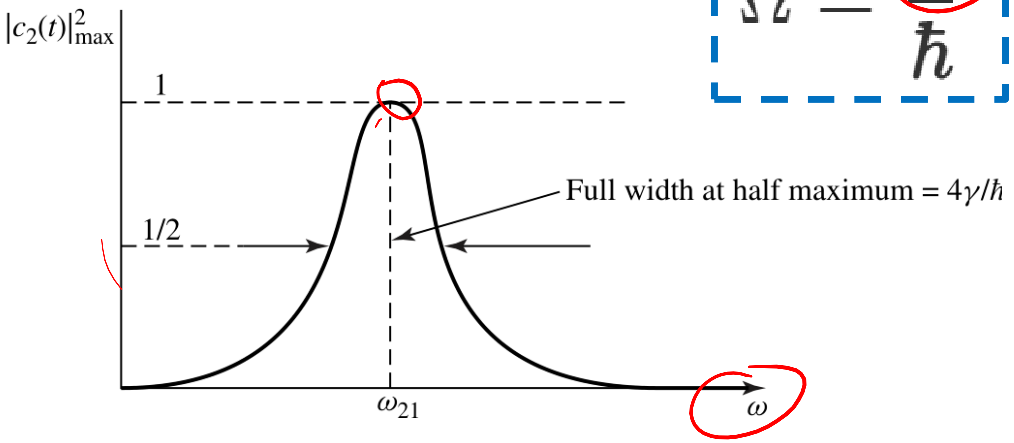
$$|c_1(t)|^2 = 1 - |c_2(t)|^2$$

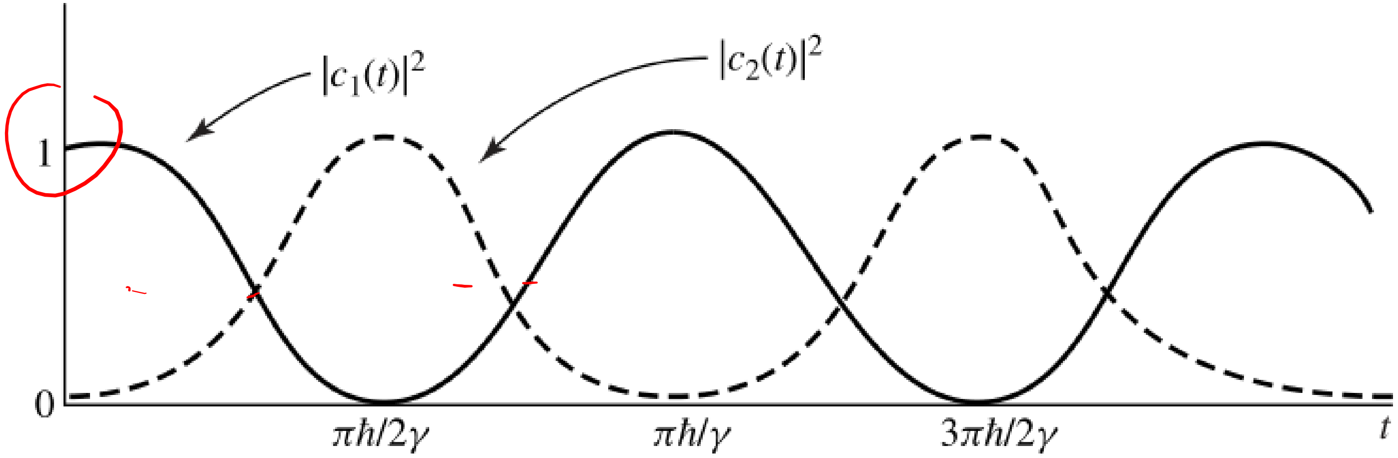
Frequência de Rabi

$$\Omega = \sqrt{\left(\frac{\gamma^2}{\hbar^2}\right) + \frac{(\omega-\omega_{21})^2}{4}}$$

Ressonância

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

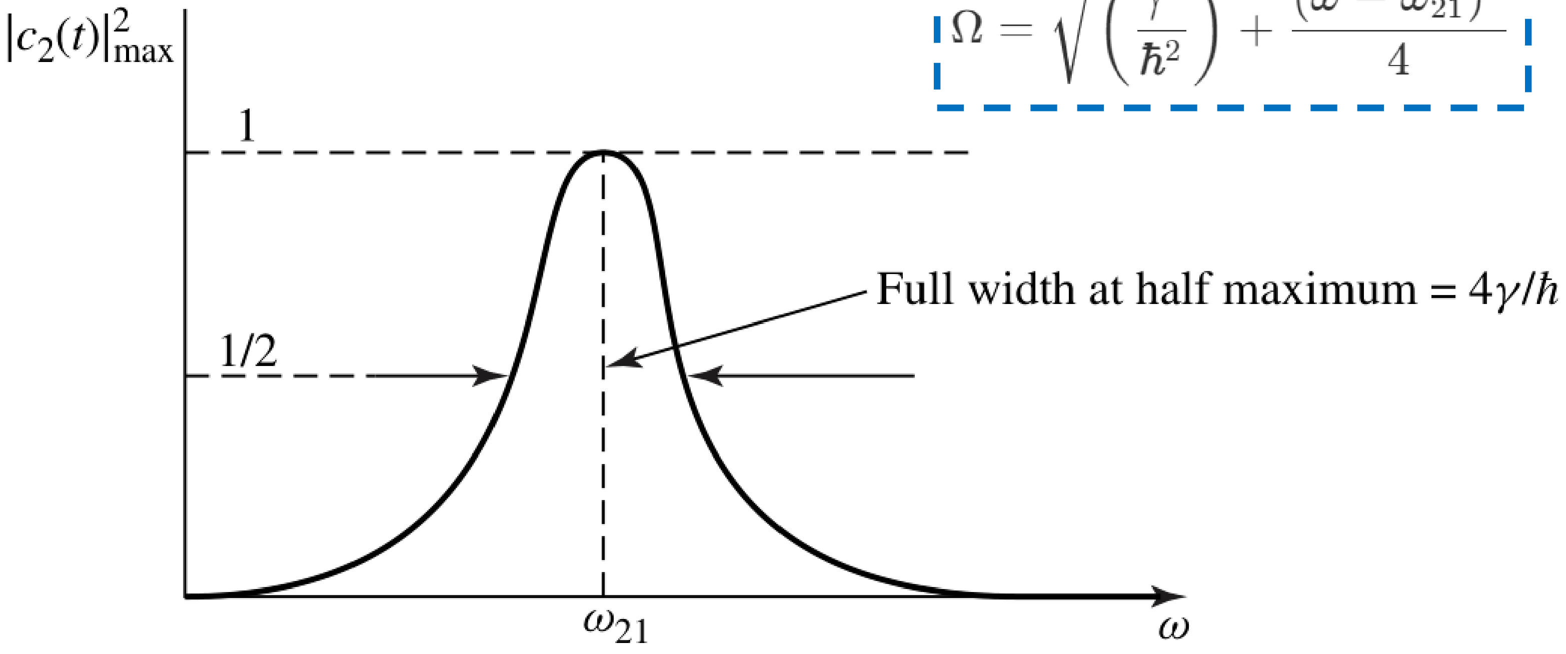




Sistema dois níveis (osc. de Rabi)

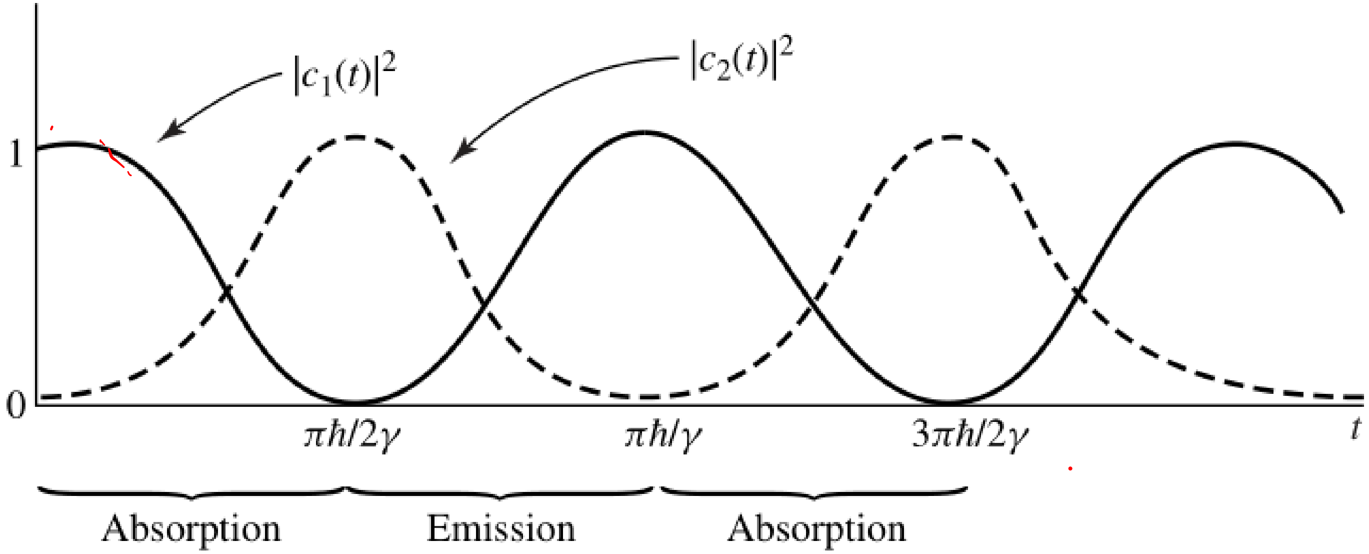
Frequência de Rabi

$$\boxed{\Omega = \sqrt{\left(\frac{\gamma^2}{\hbar^2}\right) + \frac{(\omega - \omega_{21})^2}{4}}}$$



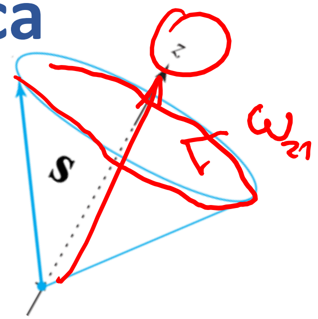
Ressonância

$$\boxed{\Omega = \frac{\gamma}{\hbar}}$$



Ex. Sistema dois níveis (osc. de Rabi) - spin & ressonância magnética

$\vec{S} = (S_x, S_y, S_z)$ $\hat{S}_i = \frac{\hbar}{2}\hat{\sigma}_i$



$$\boxed{\mathbf{B} = B_0\hat{\mathbf{z}} + B_1(\hat{\mathbf{x}}\cos\omega t + \hat{\mathbf{y}}\sin\omega t)}$$

$$\boldsymbol{\mu} = \frac{e}{m_e c}\mathbf{S}$$

$\hat{H} = -\vec{\mu}\cdot B$

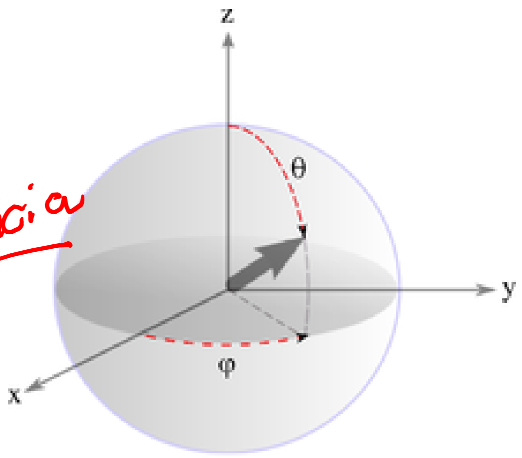
$$H_0 = \underbrace{\left(\frac{e\hbar B_0}{2m_e c}\right)}_{-E_0}(|+\rangle\langle+| - |-\rangle\langle-|)$$

$$V(t) = -\underbrace{\left(\frac{e\hbar B_1}{2m_e c}\right)}_{\gamma}[\cos\omega t(|+\rangle\langle-| + |-\rangle\langle+|) + \sin\omega t(-i|+\rangle\langle-| + i|-\rangle\langle+|)]$$

$$\boxed{\begin{aligned} |+\rangle &\to |2\rangle \\ |-\rangle &\to |1\rangle \end{aligned}}$$

$$\boxed{\begin{aligned} &E_0 = \frac{-e\hbar B_0}{2m_e c}; \quad \overset{\gamma}{\cancel{V_1}} = \frac{-e\hbar B_1}{2m_e c} \\ &E_1 = -E_0; \quad E_2 = E_0 \end{aligned}}$$

$$V(t) = \begin{pmatrix} 0 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & 0 \end{pmatrix}, \quad H = \begin{pmatrix} -E_0 & \gamma e^{i\omega t} \\ \gamma e^{-i\omega t} & E_0 \end{pmatrix}$$



Ressonância

$$\boxed{\omega \to \omega_{21} = \frac{|e|B_0}{m_e c}}$$

Larmor

$$\boxed{\gamma = \frac{-e\hbar B_1}{2m_e c}}$$

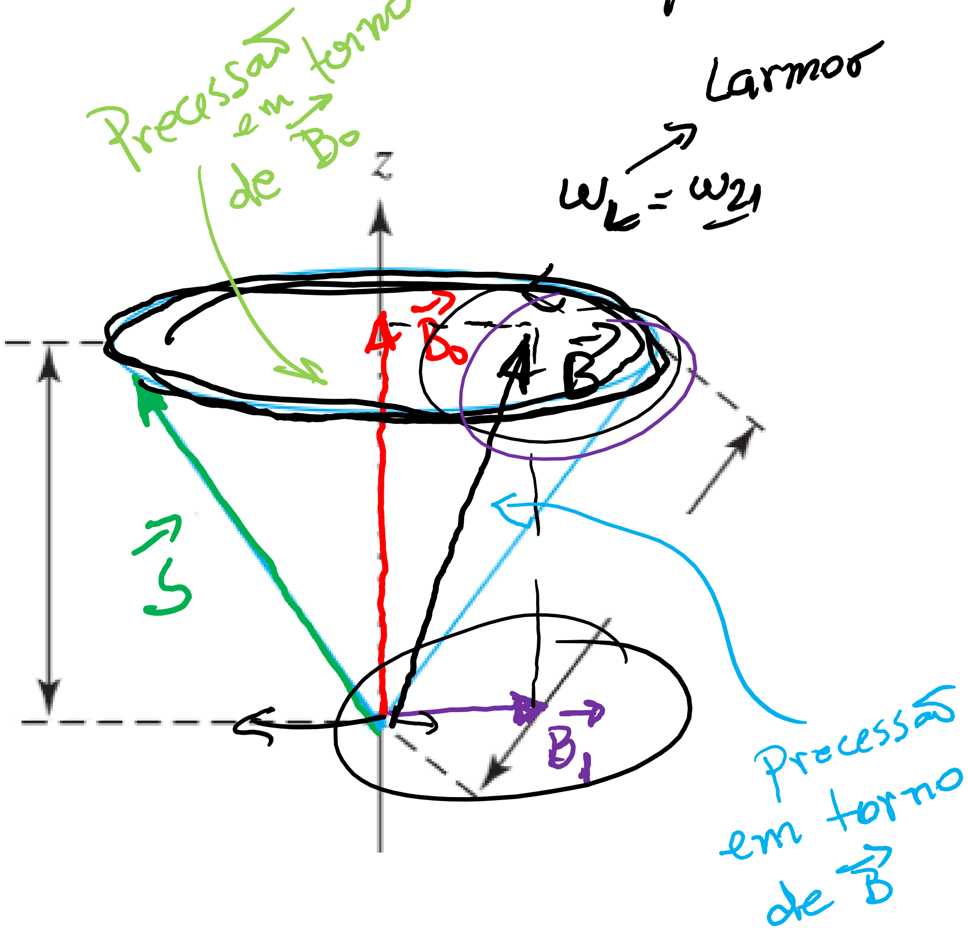
Interação

$$\boxed{\Omega = \frac{\gamma}{\hbar} \ll \omega_{21}}$$

Frequência de Rabi

Quiz

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



$\langle 1|2\rangle = 0$