GABARITO LISTA X

1.) Considere um sistema de dois níveis, cuja Hamiltoniana é

$$H = H_0 + H_1$$
$$= -\alpha B_0 \sigma_3 - \alpha B_1 [\sigma_1 \cos\omega t + \sigma_2 \sin\omega t].$$

Inicialmente $(t=0)$ o sistema encontra-se no estado

$$\psi(t=0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

a) Obtenha a solução exata desse problema.

Devemos resolver a equação de Schrödinger

$$i\hbar \frac{\partial}{\partial t}|\psi(t)\rangle = H|\psi(t)\rangle.$$

Escrevendo

$$|\psi(t)\rangle = C_1(t)|+\rangle + C_2(t)|-\rangle,$$

sendo

$$|+\rangle \to \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \qquad |-\rangle \to \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

a base dos autoestados de H_0.

Portanto, nessa base

$$\Psi(t) = \begin{pmatrix} \langle + | \psi(t) \rangle \\ \langle - | \psi(t) \rangle \end{pmatrix} = \begin{pmatrix} C_1(t) \\ C_2(t) \end{pmatrix},$$

e a equação de Schrödinger fica

$$i\hbar \frac{\partial}{\partial t} \begin{pmatrix} C_1(t) \\ C_2(t) \end{pmatrix} = - \begin{pmatrix} \alpha B_0 & \alpha B_1 \overbrace{(\cos \omega t - i \sin \omega t)}^{e^{-i\omega t}} \\ \alpha B_1 e^{i\omega t} & -\alpha B_0 \end{pmatrix} \begin{pmatrix} C_1(t) \\ C_2(t) \end{pmatrix}$$

$$= - \begin{pmatrix} \alpha B_0 C_1(t) + \alpha B_1 e^{-i\omega t} C_2(t) \\ \alpha B_1 e^{i\omega t} C_1(t) - \alpha B_0 C_2(t) \end{pmatrix},$$

ou seja, temos o sistema de equações,

$$i\hbar \frac{\partial C_1}{\partial t} = -\alpha B_0 C_1 - \alpha B_1 e^{-i\omega t} C_2(t), \qquad (1)$$

$$i\hbar \frac{\partial C_2}{\partial t} = -\alpha B_1 e^{i\omega t} C_1 + \alpha B_0 C_2. \qquad (2),$$

definamos

$$C_1(t) = e^{+\frac{i}{\hbar}\alpha B_0 t} x(t) \Rightarrow x(t) = e^{-\frac{i}{\hbar}\alpha B_0 t} C_1(t)$$

$$C_2(t) = e^{-\frac{i}{\hbar}\alpha B_0 t} y(t) \Rightarrow y(t) = e^{\frac{i}{\hbar}\alpha B_0 t} C_2(t)$$

tal que

$$\frac{\partial x}{\partial t} = \frac{\partial}{\partial t}\left(e^{-\frac{i\alpha B_0 t}{\hbar}} C_1(t)\right)$$

$$= -\frac{i}{\hbar}\alpha B_0 e^{-\frac{i\alpha B_0 t}{\hbar}} C_1(t) + e^{-\frac{i\alpha B_0 t}{\hbar}} \frac{\partial}{\partial t} C_1(t)$$

$$= \cancel{-\frac{i}{\hbar}\alpha B_0 e^{-\frac{i\alpha B_0 t}{\hbar}} C_1(t)} + e^{-\frac{i\alpha B_0 t}{\hbar}} \cdot \frac{1}{i\hbar}\left(-\cancel{\alpha B_0 C_1} - \alpha B_1 e^{-i\omega t} C_2(t)\right)$$

$$= +\frac{i}{\hbar} e^{-\frac{i\alpha B_0 t}{\hbar}} e^{-i\omega t} \alpha B_1 C_2(t) \qquad \text{fazendo } \hbar = 1.$$

$$= i\, e^{-i(\alpha B_0 + \omega)t} \alpha B_1\, y(t)\, e^{-i\alpha B_0 t}$$

$$= i\, e^{-i(2\alpha B_0 + \omega)t} \alpha B_1\, y(t)$$

$$\frac{\partial y}{\partial t} = \frac{\partial}{\partial t}\left(e^{i\alpha B_0 t} C_2(t)\right)$$

$$= i\alpha B_0 t\, e^{i\alpha B_0 t} C_2(t) + e^{i\alpha B_0 t} \frac{\partial C_2(t)}{\partial t}$$

$$= \cancel{i\alpha B_0 t\, e^{i\alpha B_0 t} C_2} + e^{i\alpha B_0 t}\left(+\frac{i}{\hbar}\alpha B_1 e^{i\omega t} C_1(t) - \cancel{i\alpha B_0 C_2}\right)$$

$$= i\alpha B_1 e^{i(\alpha B_0 + \omega)t} C_1(t)$$

$$= i\alpha B_1 e^{i(2\alpha B_0 + \omega)t} x(t)$$

Temos o novo sistema,

$$\frac{\partial x}{\partial t} = i\alpha B_1 e^{-i(2\alpha B_0 + \omega)t} y(t), \quad \frac{\partial y}{\partial t} = i\alpha B_1 e^{i(2\alpha B_0 + \omega)t} x(t)$$

derivando a primeira equação com relação ao tempo,

•)
$$\frac{\partial^2 x}{\partial t^2} = i\alpha B_1 \left\{ -i(2\alpha B_0 + \omega) e^{-i(2\alpha B_0+\omega)t} y(t) + e^{-i(2\alpha B_0+\omega)t} \frac{\partial y}{\partial t} \right\}$$

$$= i\alpha B_1 \left\{ -i(2\alpha B_0 + \omega) \frac{\partial x}{\partial t} \frac{1}{i\alpha B_1} + i\alpha B_1 e^{-i(2\alpha B_0+\omega)t} e^{i(2\alpha B_0+\omega)t} x \right\}$$

$$= -i(2\alpha B_0 + \omega) \frac{\partial x}{\partial t} - \alpha^2 B_1^2 x$$

$$\frac{\partial^2 x}{\partial t^2} + i(2\alpha B_0 + \omega) \frac{\partial x}{\partial t} + \alpha^2 B_1^2 x = 0,$$

•) Similarmente,

$$\frac{\partial^2 y}{\partial t^2} = i\alpha B_1 \left\{ i(2\alpha B_0 + \omega) \underbrace{e^{+i(2\alpha B_0+\omega)} x(t)}_{\frac{1}{i\alpha B_1}\frac{\partial y}{\partial t}} + e^{i(2\alpha B_0+\omega)t} \frac{\partial x}{\partial t} \right\}$$

$$= i\alpha B_1 \left\{ \frac{i(\alpha B_0 \cdot 2 + \omega)}{i\alpha B_1} \frac{\partial y}{\partial t} + e^{i(2\alpha B_0+\omega)t} \cdot i\alpha B_1 e^{-i(2\alpha B_0+\omega)t} y \right\}$$

$$= i(2\alpha B_0 + \omega) \frac{\partial y}{\partial t} - \alpha^2 B_1^2 y$$

$$\frac{\partial^2 y}{\partial t^2} - i(2\alpha B_0 + \omega) \frac{\partial y}{\partial t} + \alpha^2 B_1^2 y = 0$$

As condições iniciais são obtidas considerando

$$C_1(0) = 1 \quad , \quad C_2(0) = 0,$$

isto implica que

$$x(0) = 1, \qquad y(0) = 0,$$

$$x'(0) = 0, \qquad y'(0) = i\alpha B_1.$$

Definindo

$$\omega_1 = 2\alpha B_0 + \omega,$$

$$\beta = \alpha B_1,$$

obtemos as soluções

∘) $$C_1(t) = e^{i\alpha B_0 t}\left\{\frac{i\,\omega_1}{\sqrt{4\beta^2+\omega_1^2}}\, e^{-\frac{i}{2}\omega_1 t}\,\mathrm{Sin}\left(\frac{1}{2}\sqrt{4\beta^2+\omega_1^2}\,t\right)\right.$$

$$\left. + \, e^{-\frac{i}{2}\omega_1 t}\,\mathrm{Cos}\left(\frac{1}{2}\sqrt{4\beta^2+\omega_1^2}\,t\right)\right\}$$

$$= e^{-\frac{i\omega t}{2}}\left\{\frac{i\,\omega_1}{\sqrt{4\beta^2+\omega_1^2}}\,\mathrm{Sin}\left[\frac{1}{2}\sqrt{4\beta^2+\omega_1^2}\,t\right] + \mathrm{Cos}\left(\frac{1}{2}\sqrt{4\beta^2+\omega_1^2}\,t\right)\right\}$$

∘) $$C_2(t) = e^{\frac{i\omega t}{2}}\,\frac{\mathrm{Sin}\left[\frac{1}{2}t\sqrt{4\beta^2+\omega_1^2}\right]}{\sqrt{4\beta^2+\omega_1^2}}\cdot 2i\beta$$

Notemos que $|C_1(t)|^2 + |C_2(t)|^2 = 1.$

Explícitamente

$$|C_1(t)|^2 = \cos^2\left(\frac{1}{2}\sqrt{4\beta^2+\omega_i^2}\,t\right) + \frac{\omega_i^2}{4\beta^2+\omega_i^2}\sin^2\left(\frac{1}{2}\sqrt{4\beta^2+\omega_i^2}\,t\right)$$

$$|C_2(t)|^2 = \frac{4\beta^2}{4\beta^2+\omega_i^2}\sin^2\left(\frac{1}{2}\sqrt{4\beta^2+\omega_i^2}\,t\right)$$

b) Utilizando teoria de perturbação dependente do temp até primeira ordem obtenha uma solução aproximada do problema

Os coeficientes de transição até primeira ordem são

$$C_n^{(1)}(t) = -\frac{i}{\hbar}\int_0^t dt'\, e^{i\frac{E_n-E_i}{\hbar}t'} \langle n|V(t')|i\rangle$$

Para o caso em consideração

$$H|\pm\rangle = E_\pm|\pm\rangle \Rightarrow E_\pm = \mp\alpha B_0,$$

além disso,

◦) $$\langle +|V(t)|+\rangle = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}0 & -\alpha B_1 e^{-i\omega t}\\ -\alpha B_1 e^{i\omega t} & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = 0$$

◦) $$\langle +|V(t)|-\rangle = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}0 & -\alpha B_1 e^{-i\omega t}\\ -\alpha B_1 e^{i\omega t} & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix}$$

$$= -\alpha B_1 e^{i\omega t}$$

$\circ)$ $$\langle - | V(t) | + \rangle = -\alpha B_1 e^{-i\omega t} .$$

Portanto

$\circ)$ $$C_1^{(1)}(t) = 0$$

$\circ)$ $$C_2^{(1)}(t) = -i \int_0^t dt' \, e^{i 2\alpha B_0 t'} (-\alpha B_1) e^{i\omega t'}$$

$$= \underbrace{i\alpha B_1}_{\beta} \int_0^t dt' \, e^{i\underbrace{(2\alpha B_0 + \omega)}_{\Omega_1} t'}$$

$$= i\beta \frac{1}{i\Omega_1} e^{i\Omega_1 t'} \Big|_0^t = \frac{\beta}{\Omega_1} \left\{ e^{i\Omega_1 t} - 1 \right\}$$

$$= \frac{\beta}{\Omega_1} e^{\frac{i}{2}\Omega_1 t} \left\{ e^{\frac{i}{2}\Omega_1 t} - e^{-\frac{i}{2}\Omega_1 t} \right\}$$

$$= \frac{\beta}{\Omega_1} e^{\frac{i}{2}\Omega_1 t} \, 2i \sin \frac{\Omega_1}{2} t ,$$

A probabilidade é

$$|C_2^{(1)}(t)|^2 = \frac{4\beta^2}{\Omega_1^2} \sin^2 \frac{\Omega_1}{2} t .$$

c) Comparando os resultados anteriores, discuta a validade da aproximação.

Tomemos o limite

$$\Omega \gg \beta$$

na solução exata,

$$|C_2(t)|^2 \simeq \frac{4\beta^2}{\Omega^2} \sin^2\left(\frac{\Omega}{2}t\right),$$

portanto, obtemos o resultado da teoria de perturbação. o limite implica que

$$2\alpha B_0 + \omega \gg B_1 \alpha,$$

ou seja

$$B_1 \ll 2B_0 + \frac{\omega}{\alpha}$$

$$\frac{1}{2}\left(B_1 - \frac{\omega}{\alpha}\right) \ll B_0 .$$

Assim, a teoria de perturbações somente será valida nessa situação.

2.) Obtenha a regra áurea de Fermi utilizando teoria de Perturbações dependente do tempo até segunda ordem para uma perturbação constante.

Os coeficientes dependentes do tempo até segunda ordem são

$$C_n = C_n^{(0)} + C_n^{(1)} + C_n^{(2)},$$

sendo

$|i\rangle \to$ inicial

$|n\rangle \to$ final

$$C_n^{(0)} = \langle n|i\rangle = \delta_{ni}$$

$$C_n^{(1)} = -\frac{i}{\hbar}\int_{t_0}^{t} dt'\, e^{\frac{i}{\hbar}(E_n-E_i)t'} \langle n|V(t')|i\rangle$$

$$C_n^{(2)} = \left(-\frac{i}{\hbar}\right)^2 \sum_m \int_{t_0}^{t} dt' \int_{t_0}^{t'} dt''\, e^{\frac{i}{\hbar}(E_n-E_m)t'}\, e^{\frac{i}{\hbar}(E_m-E_i)t''} \langle n|V(t')|m\rangle \langle m|V(t'')|i\rangle.$$

Considerando o caso

$$V(t) = V_0\, e^{\frac{\eta t}{\hbar}},$$

temos que $(t_0 \to -\infty)$

∘)
$$C_n^{(1)} = -\frac{i}{\hbar}\int_{-\infty}^{t} dt'\, e^{\frac{i}{\hbar}(E_n-E_i)t'} \langle n|V_0|i\rangle e^{\frac{\eta t'}{\hbar}}$$

$$= -\frac{i}{\hbar}\langle n|V_0|i\rangle \int_{-\infty}^{t} dt'\, e^{\frac{i}{\hbar}(E_n-E_i-i\eta)t'} = -\frac{i}{\hbar}\langle n|V_0|i\rangle \frac{-i}{\frac{1}{\hbar}(E_n-E_i-i\eta)} \cdot \left\{ e^{\frac{i}{\hbar}(E_n-E_i-i\eta)t} \right\}$$

$$C_n^{(1)}(t) = - \frac{\exp\left\{\frac{i}{\hbar}(E_n - E_i - i\eta)t\right\}}{E_n - E_i - i\eta} \langle n|V_0|i\rangle$$

-) $$C_n^{(2)}(t) = \left(-\frac{i}{\hbar}\right)^2 \sum_m \int_{-\infty}^{t} dt' \, e^{\frac{i}{\hbar}(E_n - E_m)t'} \int_{-\infty}^{t'} dt'' \, e^{\frac{i}{\hbar}(E_m - E_i)t''} \, e^{\frac{\eta t'}{\hbar}} e^{\frac{\eta t''}{\hbar}} \langle n|V_0|m\rangle \langle m|V_0|i\rangle$$

$$= \left(-\frac{i}{\hbar}\right)^2 \sum_m \langle n|V_0|m\rangle\langle m|V_0|i\rangle \int_{-\infty}^{t} dt' e^{\frac{i}{\hbar}(E_n - E_m - i\eta)t'} \underbrace{\int_{-\infty}^{t'} dt'' \, e^{\frac{i}{\hbar}(E_m - E_i - i\eta)t''}}_{\frac{-i\exp\left\{\frac{i}{\hbar}(E_m - E_i - i\eta)t'\right\}}{(E_m - E_i - i\eta)\frac{1}{\hbar}}}$$

$$= \left(-\frac{i}{\hbar}\right)^2 \sum_m \frac{\langle n|V_0|m\rangle\langle m|V_0|i\rangle}{\frac{1}{\hbar}(E_m - E_i - i\eta)}(-i) \underbrace{\int_{-\infty}^{t} dt' \, e^{\frac{i}{\hbar}(E_n - \cancel{E_m} - i\eta + \cancel{E_m} - E_i - i\eta)t'}}_{\frac{-i}{\frac{1}{\hbar}(E_n - E_i - 2i\eta)}\exp\left\{\frac{i}{\hbar}(E_n - E_i - 2i\eta)t\right\}}$$

$$= \left(-\frac{i}{\cancel{\hbar}}\right)^2 \frac{-1}{\frac{1}{\cancel{\hbar}}(E_n - E_i - 2i\eta)} \sum_m \frac{\langle n|V_0|m\rangle\langle m|V_0|i\rangle}{\frac{1}{\cancel{\hbar}}(E_m - E_i - i\eta)} \exp\left\{\frac{i}{\hbar}(E_n - E_i - 2i\eta)t\right\}$$

$$= \frac{\exp\left\{\frac{i}{\hbar}(E_n - E_i - 2i\eta)t\right\}}{E_n - E_i - 2i\eta} \sum_m \frac{\langle n|V_0|m\rangle\langle m|V_0|i\rangle}{E_m - E_i - i\eta}$$

Portanto, considerando $n \neq i$,

$$C_n = -\frac{\exp\left\{\frac{i}{\hbar}(E_n - E_i - i\eta)t\right\}}{E_n - E_i - i\eta}\langle n|V_0|i\rangle$$

$$+\frac{\exp\left\{\frac{i}{\hbar}(E_n - E_i - 2i\eta)t\right\}}{E_n - E_i - 2i\eta}\sum_m \frac{\langle n|V_0|m\rangle\langle m|V_0|i\rangle}{E_m - E_i - i\eta}$$

$$= \frac{\exp\left\{\frac{i}{\hbar}(E_n - E_i - i\eta)t\right\}}{E_n - E_i - i\eta}\left\{\langle n|V_0|i\rangle - \frac{e^{\frac{\eta t}{\hbar}}(E_n - E_i - i\eta)}{E_n - E_i - 2i\eta}\sum_m \frac{\langle n|V_0|m\rangle\langle m|V_0|i\rangle}{E_m - E_i - i\eta}\right\}$$

A taxa de transição é obtida mediante,

$$\frac{dP_{in}}{dt} = \frac{d}{dt}|C_n(t)|^2$$

$$= \frac{d}{dt}\left\{\frac{e^{\frac{2\eta t}{\hbar}}}{(E_n - E_i)^2 + \eta^2}\left|\langle n|V_0|i\rangle + e^{\eta t}\frac{(E_n - E_i - i\eta)}{E_n - E_i - 2i\eta}\sum_m \frac{\langle n|V_0|m\rangle\langle m|V_0|i\rangle}{E_m - E_i - i\eta}\right|^2\right.$$

$$= \frac{2\eta\, e^{\frac{2\eta t}{\hbar}}}{\hbar[(E_n - E_i)^2 + \eta^2]}\left|\langle n|V_0|i\rangle - \frac{e^{\eta t}(E_n - E_i - i\eta)}{E_n - E_i - 2i\eta}\sum_m \frac{\langle n|V_0|m\rangle\langle m|V_0|i\rangle}{E_m - E_i - i\eta}\right|^2$$

$$+ \frac{e^{\frac{2\eta t}{\hbar}}}{(E_n - E_i)^2 + \eta^2}\cdot 2\left|\langle n|V_0|i\rangle - \frac{e^{\eta t}(E_n - E_i - i\eta)}{E_n - E_i - 2i\eta}\sum_m \frac{\langle n|V_0|m\rangle\langle m|V_0|i\rangle}{E_m - E_i - i\eta}\right|$$

$$\cdot \frac{d}{dt}\left(-e^{\eta t}\frac{(E_n - E_i - i\eta)}{E_n - E_i - 2i\eta}\sum_m \frac{\langle n|V_0|m\rangle\langle m|V_0|i\rangle}{E_m - E_i - i\eta}\right)$$

Tomando o limite $\eta \to 0$, o segundo termo cancela, enquanto que o primeiro da

$$\frac{dP_{i\to n}}{dt} = \frac{2\pi}{\hbar}\,\delta(E_n - E_i)\left|\langle n|V_0|i\rangle - \sum_m \frac{\langle n|V_0|m\rangle\langle m|V_0|i\rangle}{E_m - E_i}\right|^2 .$$

A regra de ouro de Fermi é

$$\Gamma_{i\to n} \doteq \frac{2\pi}{\hbar}\,\rho(E_i)\left|\langle n|V_0|i\rangle - \sum_m \frac{\langle n|V_0|m\rangle\langle m|V_0|i\rangle}{E_m - E_i}\right|^2$$