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QMIII - Tutorial 2

Q1)
$H_0 = E_1 |1\rangle \langle 1| + E_2 |2\rangle \langle 2|$.
$H_0 = \begin{bmatrix} E_1 & 0 \\ 0 & E_2 \end{bmatrix}$ in basis $\{|1\rangle, |2\rangle\}$
$V(t)_s = \gamma e^{i\omega t} |1\rangle \langle 2| + \gamma e^{-i\omega t} |2\rangle \langle 1|$
Interaction picture :
$|\Psi(t)\rangle_I = e^{i\hat{H}t/\hbar} |\Psi(t)\rangle_s$
$V(t)_I = e^{i\hat{H}t/\hbar} V_s e^{-i\hat{H}t/\hbar} = \gamma \begin{bmatrix} 0 & e^{i(\omega-\omega_{21})t} \\ e^{-i(\omega-\omega_{21})t} & 0 \end{bmatrix}$
where $\omega_{21} = \dfrac{E_2 - E_1}{\hbar}$

Schrodinger equation :
$i\hbar \dfrac{\partial |\Psi(t)\rangle_I}{\partial t} = V(t)_I |\Psi(t)\rangle_I$
Take $|\Psi(t)\rangle = \begin{bmatrix} c_1(t) \\ c_2(t) \end{bmatrix}$
$\implies i\hbar \dot{c}_k(t) = \sum_n V_{kn}(t) e^{i\omega_{mn}t} c_n(t)$

i)
$i\hbar \dfrac{\partial \vec{c}(t)}{\partial t} = \gamma \begin{bmatrix} 0 & e^{i(\omega-\omega_{21})t} \\ e^{-i(\omega-\omega_{21})t} & 0 \end{bmatrix} \vec{c}(t)$
$i\hbar \begin{bmatrix} \dot{c}_1(t) \\ \dot{c}_2(t) \end{bmatrix} = \begin{bmatrix} e^{i(\omega-\omega_{21})t} c_2(t) \\ e^{-i(\omega-\omega_{21})t} c_1(t) \end{bmatrix}$
Taking another derivative ,
$i\hbar \begin{bmatrix} \ddot{c}_1(t) \\ \ddot{c}_2(t) \end{bmatrix} = \gamma \begin{bmatrix} e^{i(\omega-\omega_{21})t} \dot{c}_2(t) + i(\omega - \omega_{21}) e^{i(\omega-\omega_{21})t} c_2(t) \\ e^{-i(\omega-\omega_{21})t} \dot{c}_1(t) - i(\omega - \omega_{21}) e^{-i(\omega-\omega_{21})t} c_1(t) \end{bmatrix}$

From the above 2 equations, we can construct a second order ode for $c_2(t)$.
$\ddot{c}_2(t) + i(\omega - \omega_{21})\dot{c}_2(t) + \dfrac{\gamma^2}{\hbar^2} c_2(t) = 0$
Solving this we get the expression mentioned in the appendix,
$c_2(t) = A e^{at/2} \sin \Omega t$
where,
$a = i(\omega - \omega_{21}), \Omega = [\dfrac{\gamma^2}{\hbar^2} + \dfrac{(\omega - \omega_{21})^2}{4}]^{1/2}$
$A = \dfrac{\gamma}{\hbar \Omega}$
The Probability of finding the state in the excited state therefore is,
$|c_2(t)|^2 = \dfrac{\gamma^2}{\gamma^2 + \hbar^2(\omega^2 - \omega_{21}^2)/4} \sin^2 \Omega t$

ii)
When using perturbation theory,
$c_2(t) = c_2^{(0)}(t) + c_2^{(1)}(t) + \dots$
$c_2^{(0)}(t) = 0$ is our initial condition as it is the unperturbed term.

The first order perturbation is, $c_2^{(1)}(t) = -\frac{i\gamma}{\hbar}\int_{t_0}^{t} dt' e^{i\omega_{21}t'} V_{21}(t')_s$

$$c_2^1(t) = -\frac{i\gamma}{\hbar}\int_{t_0}^{t} dt' e^{-i(\omega-\omega_{21})t'}$$
$$= \frac{\gamma}{\hbar(\omega-\omega_{21})}(e^{-i(\omega-\omega_{21})t} - e^{-i(\omega-\omega_{21})t_0})$$

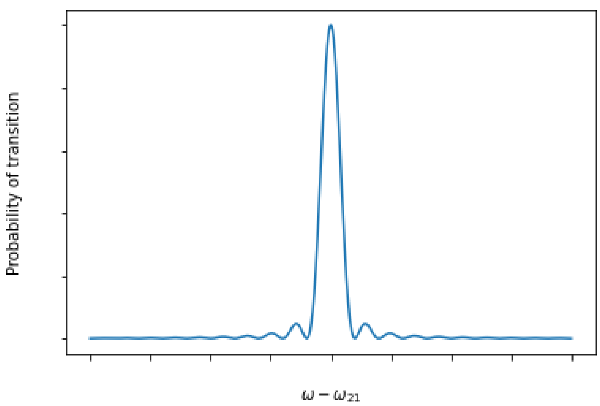
Probability
$$|c_2(t)|^2 \simeq |c_2^1(t)|^2$$
$$= \frac{\gamma^2}{\hbar^2(\omega-\omega_{21})^2}(2 - (e^{-i(\omega-\omega_{21})(t-t_0)} + e^{i(\omega-\omega_{21})(t-t_0)}))$$
$$|c_2(t)|^2 \simeq \frac{\gamma^2}{\hbar^2(\omega-\omega_{21})^2/4}\sin^2((\omega-\omega_{21})t/2)$$

Comparing this result to the exact one, we see that the requirement for perturbation is

$$\frac{\gamma}{\hbar(\omega-\omega_{21})} \ll 1$$

iii)
$P(1 \to 2) = |c_2(t)|^2 \propto \frac{\sin^2((\omega-\omega_{21})t/2)}{(\omega-\omega_{21})^2}$
The minima are as $\sin(x) = 0$ and the maxima at $\tan(x) = x$ where $x = (\omega-\omega_{21})t/2$
Therefore, the probability drops to 0 at $\frac{(\omega-\omega_{21})}{2}t = n\pi$

The probability becomes maximum when ω which is the frequency of perturbation becomes nearly equal to the energy difference between the eigenstates of the two level system(non-perturbing Hamiltonian).



Q3)
$V(x,y,z) = 0$ for $0 < x < a,\ 0 < y < 2a,\ 0 < z < 4a$
$V = \infty$ everywhere else.
i)
Schrodinger eq.
$$-\frac{\hbar^2}{2m}\nabla^2\Psi = E\Psi$$

Seperation of variables, $\Psi = \Psi_{n_x}(x)\Psi_{n_y}(y)\Psi_{n_z}(z)$
This seperates the Schrodinger equation into three seperate ODEs which give the solution for a particle in a box,

$$\Psi = \sqrt{\frac{8}{L_xL_yL_z}}\sin\left(\frac{n_x\pi x}{L_x}\right)\sin\left(\frac{n_y\pi y}{L_y}\right)\sin\left(\frac{n_z\pi z}{L_z}\right)$$
and the energy eigenstates,
$$E_{n_xn_yn_z} = \frac{\hbar^2}{8m}\left(\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2}\right)$$

As $L_x = a,\ L_y = 2a,\ L_z = 4a,$

$$\Psi(x,y,z) = \sqrt{\frac{1}{a^3}}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{2a}\right)\sin\left(\frac{n_z\pi z}{4a}\right)$$
$$E_{n_xn_yn_z} = \frac{\hbar^2}{8ma^2}\left(n_x^2 + \frac{n_y^2}{4} + \frac{n_z^2}{16}\right) \text{ for } n_x, n_y, n_z \in \mathbb{N}$$

ii)
$$E_{ground} = E_{111} = \frac{\hbar^2}{8ma^2}\left(1 + \frac{1}{4} + \frac{1}{16}\right)$$
$$E_{\text{first excited}} = E_{112} = \frac{\hbar^2}{8ma^2}\left(1 + \frac{1}{4} + \frac{4}{16}\right)$$

$$\Psi_{111} = \sqrt{\frac{1}{a^3}}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{\pi y}{2a}\right)\sin\left(\frac{\pi z}{4a}\right)$$
$$\Psi_{112} = \sqrt{\frac{1}{a^3}}\sin\left(\frac{\pi x}{a}\right)\sin\left(\frac{\pi y}{2a}\right)\sin\left(\frac{\pi z}{2a}\right)$$

The Transition amplitude from the ground to the first excited state by using time dependent perturbation theory is,

$$c^{(1)}_{1\to 2}(t\to\infty) = -\frac{i}{\hbar}\int_{\infty}^{\infty} dt' e^{i\omega_{21}t'}V_{21}(t')$$
where $\omega_{21} = \dfrac{E_{112} - E_{111}}{\hbar} = \dfrac{3\pi^2\hbar}{32ma^2}$
$V_{21}(t) = \langle 1,1,2|\, V(t)\, |1,1,1\rangle$

$$V_{21}(t) = \langle 1,1,2|\, V(t)\, |1,1,1\rangle$$
$$= \frac{1}{a^3} V_0 \int d^3x \sin^2(\frac{\pi x}{a}) \sin^2(\frac{\pi y}{2a}) \sin^2(\frac{\pi z}{2a}) \sin^2(\frac{\pi z}{4a}) xz e^{-t^2}$$
$$= \frac{e^{-t^2}}{a^3} V_0 \int_0^a dx \sin^2(\frac{\pi x}{a}) x \int_0^{2a} dy \sin^2(\frac{\pi y}{2a}) \int_0^{4a} \sin^2(\frac{\pi z}{2a}) \sin^2(\frac{\pi z}{4a}) z$$
$$= -\frac{32 a^2 V_0}{9\pi^2} e^{-t^2}$$

$$c^{(1)}_{1\to 2}(t \to \infty) = i \frac{32 a^2 V_0}{9\pi^2 \hbar} \int_{-\infty}^{\infty} dt' e^{i\omega_{21} t' - t'^2}$$

Using the identity, $\int_{-\infty}^{\infty} dt e^{i\omega t - t^2/\tau} = \sqrt{\pi}\tau e^{-\omega^2\tau^2/4}$

$$c^{(1)}_{1\to 2}(t \to \infty) = i \frac{32 a^2 V_0}{9\pi^2 \hbar} \sqrt{\pi} e^{-\omega^2/4}$$
$$P_{g\to ex} \simeq (\frac{32 a^2 V_0}{9\pi^2 \hbar})^2 \pi e^{-\omega_{21}^2/2}$$

Q2

(i) $H = H_0 + H'(t)$.

$$\Psi(t) = \sum c_n(t)\, \psi_n\, e^{iE_n t/\hbar}.$$

$$\dot{c}_m = -\frac{i}{\hbar} \sum_n c_n H'_{mn}\, e^{i(E_m - E_n)t/\hbar}.$$

for the system starting out in state N.

$$c_N \approx 1 - \frac{i}{\hbar} \int H'_{NN}(t')\, dt'$$

$$c_M \approx -\frac{i}{\hbar} \int H'_{MN}(t)\, e^{i(E_m - E_N)t/\hbar'}\, dt' \qquad M \neq N.$$

ψ_n is eigenstate of H_0

$$H'(t) = g x^3 e^{-t/\tau}.$$

$$\psi(0) = |0\rangle.$$

$$c_n = -\frac{i}{\hbar} \int_0^{\tau} H'_{n0}(t')\, e^{i(E_m - E_n)t/\hbar}\, dt'$$

$$H_{N0} = \langle n| g x^3 e^{-t/\tau} |0\rangle.$$

$$x = \sqrt{\frac{\hbar}{2m\omega}}\,(a + a^+).$$

$$x^3 = \left(\frac{\hbar}{2m\omega}\right)^{3/2} (a^3 + a^{+3} + 2(a^2a^+ + aa^{+2}) - 2a - 2a^+ + a^+a^2 + a^+{}^2 a).$$

$$\Rightarrow x^3|0\rangle = \left(\frac{\hbar}{2m\omega}\right)^{3/2} (a^{+3} + 2(a^2a^+ + aa^{+2}) - 2a^+)|0\rangle$$

$$x^3|0\rangle = \left(\frac{\hbar}{2m\omega}\right)^{3/2} (\sqrt{6}|3\rangle + 2|1\rangle).$$

$\Rightarrow c_n(t)$ is non-zero only for. $n = 3$ & $n = 1$.

$$c_3 = -gi \frac{A^3\sqrt{6}}{\hbar} \int_0^t e^{(3i - \frac{1}{\tau})t'}\, dt' \qquad A = \sqrt{\frac{\hbar}{2m\omega}}$$

$$c_3 = \frac{-ig A^3\sqrt{6}}{\hbar(3i - \frac{1}{\tau})} \left(e^{(3i - \frac{1}{\tau})t} - 1\right).$$

$$c_1(t) = \frac{-2igA_3}{\hbar\,(i-\frac{1}{\tau})}\left(e^{(i-\frac{1}{\tau})t} - 1\right).$$

$$c_0(t) \approx 1 - \frac{i}{\hbar}\int_0^t H'_{00}(t')\,dt'$$

$$= 1 \qquad (H_{00} = 0)$$

$$|c_0(t)|^2 \approx 1 - |c_1(t)|^2 - |c_3(t)|^2$$

(this result might ~~not~~ be exact as we are using perturbation theory)

(ii) $H_1(t) = gx^2\cos(\Omega t)$

$$c_n = \frac{-i}{\hbar}\int_0^t H'_{n0}(t')\, e^{i(E_m - E_n)t'/\hbar}\,dt'$$

$$H_{n0} = \langle n|\, g x^2 \cos(\Omega t)\,|0\rangle.$$

$$\langle n|x^2|0\rangle = \langle n|\, aa^\dagger + a^\dagger a + a^2 + a^{\dagger 2}\,|0\rangle \frac{\hbar}{2m\omega}$$

$$\Rightarrow \quad H_{n0} = \frac{g\cos(\Omega t)\,\hbar}{2m\omega}\left(\langle n|0\rangle + \sqrt{2}\,\langle n|2\rangle\right)$$

$\Rightarrow$ non-zero for $n = 0$ or 2.

$$H_{00} = \frac{\hbar g\cos(\Omega t)}{2m\omega}$$

$$H_{20} = \frac{\hbar g\cos(\Omega t)}{\sqrt{2}\,m\omega}.$$

$$c_2 = \frac{-i}{\hbar}\int_0^t \frac{\hbar g\cos(\Omega t')}{\sqrt{2}\,m\omega}\, e^{i(E_2 - E_0)t'/\hbar}\,dt'$$

$$= \frac{-4ig}{\sqrt{2}\,m\omega\,(4 - \Omega^2\hbar^2)}\left(\frac{\hbar\cos(\Omega t)\,e^{2it/\hbar}}{2i} - \frac{\hbar^2\Omega\sin(\Omega t)\,e^{2it/\hbar}}{4} - \frac{\hbar}{2i}\right).$$

$$C_0(t) = 1 - \frac{i}{\hbar}\int_0^t H_{00}(t')\,dt'$$

$$= 1 - \frac{i}{\hbar}\int_0^t g\,\frac{\cos(\Omega t')\,\hbar}{2m\omega}\,dt'$$

$$\Rightarrow C_0(t) = 1 - \frac{i g}{2m\omega\Omega}\sin(\Omega t)$$