2. (Quantum Mechanics)

A system is described by a Hilbert space spanned by two orthonormal kets $|0\rangle$ and $|1\rangle$. In this basis, the matrix elements of the Hamiltonian H_0 are:

$$\begin{pmatrix} \langle 0|H_0|0\rangle & \langle 0|H_0|1\rangle \\ \langle 1|H_0|0\rangle & \langle 1|H_0|1\rangle \end{pmatrix} = \begin{pmatrix} 2\hbar\omega & 0 \\ 0 & 0 \end{pmatrix}$$

where ω is real. At time $t = 0$ the system is in state $|0\rangle$, and a perturbation, H_1, is suddenly switched on. The matrix elements of H_1 are:

$$\begin{pmatrix} \langle 0|H_1|0\rangle & \langle 0|H_1|1\rangle \\ \langle 1|H_1|0\rangle & \langle 1|H_1|1\rangle \end{pmatrix} = \begin{pmatrix} 0 & \hbar\lambda \\ \hbar\lambda & 0 \end{pmatrix}$$

where λ is real.

(a) Find the eigenvalues and (normalized) eigenvectors of the full Hamiltonian $H_0 + H_1$. You may express these eigenvalues $E_\pm$ and eigenvectors $|\mu_\pm\rangle$ in terms of ω, λ, Δ, and α, where $\Delta^2 \equiv \omega^2 + \lambda^2$ and $\alpha^2 \equiv 2\Delta(\omega + \Delta) = (\omega + \Delta)^2 + \lambda^2$. The normalized eigenvectors can be expressed in the form $(c_1/\alpha, c_2/\alpha)$ and $(-c_2/\alpha, c_1/\alpha)$. Write down expressions for c_1 and c_2.

(b) Show that the probability of finding the system in state $|1\rangle$ at time t, given that it was in state $|0\rangle$ at time 0, is given by $(\lambda^2/\Delta^2)\sin^2(\Delta t)$.

(c) By using time-dependent perturbation theory to first order, find an approximate expression for the probability in part (b).

(d) By Taylor expanding the exact probability in part (b), recover the perturbative result of part (c) in the limit that $\omega \gg \lambda$.

Solution: *Solution by Jonah Hyman (jthyman@g.ucla.edu)*

(a) If a comp problem gives you equations or defines variables that can be used to simplify your answer, use them! For this problem, those variables are Δ and α. If we don't use them at every opportunity, this problem will take too long. We will need to choose our strategy carefully to make sure the algebra is not too difficult (points at which this is done are noted throughout).

The matrix elements of the full Hamiltonian $H \equiv H_0 + H_1$ are

$$\begin{pmatrix} \langle 0|H|0\rangle & \langle 0|H|1\rangle \\ \langle 1|H|0\rangle & \langle 1|H|1\rangle \end{pmatrix} = \begin{pmatrix} 2\hbar\omega & \hbar\lambda \\ \hbar\lambda & 0 \end{pmatrix} \tag{33}$$

We need to solve the eigenvalue problem

$$H\,|\mu_\pm\rangle = E_\pm\,|\mu_\pm\rangle \tag{34}$$

We apply standard methods from linear algebra, finding the eigenvalues first and then the eigenvectors. To find the eigenvalues, find the zeros of the characteristic polynomial of the matrix H, i.e., solve the equation $\det(H - EI) = 0$ for E:

$$\begin{aligned} 0 &= \det(H - EI) \\ &= \det\begin{pmatrix} 2\hbar\omega - E & \hbar\lambda \\ \hbar\lambda & -E \end{pmatrix} \\ &= (2\hbar\omega - E)(-E) - (\hbar\lambda)(\hbar\lambda) \\ 0 &= E^2 - 2\hbar\omega E - (\hbar\lambda)^2 \end{aligned} \tag{35}$$

To solve this equation for E, use the quadratic formula:

$$E_\pm = \frac{1}{2}\left(2\hbar\omega \pm \sqrt{(2\hbar\omega)^2 + 4(\hbar\lambda)^2}\right) \tag{36}$$

Now simplify by pulling out common factors and applying the definition of $\Delta^2 \equiv \omega^2 + \lambda^2$:

$$\begin{aligned} E_\pm &= \hbar\omega \pm \hbar\sqrt{\omega^2 + \lambda^2} \\ &= \hbar\omega \pm \hbar\Delta \end{aligned}$$

$$\boxed{E_\pm = \hbar(\omega \pm \Delta)} \tag{37}$$

To find the eigenvectors, we write (34) as a matrix equation and solve. It is possible to do this in one fell swoop using the $\pm$ symbol, but because it is easy to get confused using this symbol, we will solve for $|\mu_+\rangle$ and $|\mu_-\rangle$ separately. If we write

$$\begin{pmatrix} \langle 0|\mu_+\rangle \\ \langle 1|\mu_+\rangle \end{pmatrix} \equiv \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \langle 0|\mu_-\rangle \\ \langle 1|\mu_-\rangle \end{pmatrix} \equiv \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \tag{38}$$

then (34) becomes

$$\begin{pmatrix} 2\hbar\omega & \hbar\lambda \\ \hbar\lambda & 0 \end{pmatrix}\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \hbar(\omega + \Delta)\begin{pmatrix} u_1 \\ u_2 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 2\hbar\omega & \hbar\lambda \\ \hbar\lambda & 0 \end{pmatrix}\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \hbar(\omega - \Delta)\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \tag{39}$$

We first need to write u_2 in terms of u_1 and v_2 in terms of v_1. Each matrix equation in (39) contains two equations:

$$\begin{aligned} 2\hbar\omega u_1 + \hbar\lambda u_2 &= \hbar(\omega + \Delta)u_1 & \qquad 2\hbar\omega v_1 + \hbar\lambda v_2 &= \hbar(\omega - \Delta)v_1 \\ \hbar\lambda u_1 &= \hbar(\omega + \Delta)u_2 & \hbar\lambda v_1 &= \hbar(\omega - \Delta)v_2 \end{aligned}$$

Simplifying, we get

$$(\omega - \Delta)u_1 = -\lambda u_2 \qquad (\omega + \Delta)v_1 = -\lambda v_2 \tag{40}$$

$$\lambda u_1 = (\omega + \Delta)u_2 \qquad \lambda v_1 = (\omega - \Delta)v_2 \tag{41}$$

For each pair of equations, we only need one equation to relate u_2 and v_2 to u_1 and v_1. The second equation is redundant. It's important to choose the simpler of the two equations, or else the algebra will get too complicated. But it might be unclear which equation is simplest, so let's just use both to write $|\mu_+\rangle$ and $|\mu_-\rangle$ up to an overall normalization constant. Again, we pick the normalization constants so that the rest of each vector is as simple as possible, avoiding annoying fractions.

From (40), we get the following forms for the eigenvectors, where $M_\pm$ are normalization constants:

$$\begin{pmatrix} \langle 0|\mu_+\rangle \\ \langle 1|\mu_+\rangle \end{pmatrix} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = M_+ \begin{pmatrix} -\lambda \\ \omega - \Delta \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \langle 0|\mu_-\rangle \\ \langle 1|\mu_-\rangle \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = M_- \begin{pmatrix} -\lambda \\ \omega + \Delta \end{pmatrix} \tag{42}$$

From (41), we get the following alternate forms for the eigenvectors, where $N_\pm$ are normalization constants:

$$\begin{pmatrix} \langle 0|\mu_+\rangle \\ \langle 1|\mu_+\rangle \end{pmatrix} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = N_+ \begin{pmatrix} \omega + \Delta \\ \lambda \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} \langle 0|\mu_-\rangle \\ \langle 1|\mu_-\rangle \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = N_- \begin{pmatrix} \omega - \Delta \\ \lambda \end{pmatrix} \tag{43}$$

The last step is finding the normalization constant, defined so that $\langle \mu_\pm|\mu_\pm\rangle = 1$. We now need to select the form of the eigenvectors that makes this calculation simplest:

$$1 = \langle \mu_+|\mu_+\rangle = \begin{pmatrix} u_1^* & u_2^* \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{cases} |M_+|^2(\lambda^2 + (\omega - \Delta)^2) & \text{using (42)} \\ |N_+|^2\left((\omega + \Delta)^2 + \lambda^2\right) & \text{using (43)} \end{cases} \tag{44}$$

$$1 = \langle \mu_-|\mu_-\rangle = \begin{pmatrix} v_1^* & v_2^* \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{cases} |M_-|^2(\lambda^2 + (\omega + \Delta)^2) & \text{using (42)} \\ |N_-|^2\left((\omega - \Delta)^2 + \lambda^2\right) & \text{using (43)} \end{cases} \tag{45}$$

We need only find one normalization constant for each eigenvector, so we should pay attention to which normalization constant is easier to solve for. Remember that the problem gives us a definition of $\alpha^2 \equiv (\omega + \Delta)^2 + \lambda^2$, which we have not yet used. The bottom line of (44) contains this factor, while the top line does not. Let's therefore use the top line of (44) and solve for N_+:

$$1 = |N_+|^2((\omega + \Delta)^2 + \lambda^2) = |N_+|^2\alpha^2 \Longrightarrow |N_+| = 1/\alpha \tag{46}$$

so we may write

$$\begin{pmatrix} \langle 0|\mu_+\rangle \\ \langle 1|\mu_+\rangle \end{pmatrix} = \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = N_+ \begin{pmatrix} \omega + \Delta \\ \lambda \end{pmatrix} = \begin{pmatrix} (\omega + \Delta)/\alpha \\ \lambda/\alpha \end{pmatrix} \tag{47}$$

Similarly, we should pick the top line, rather than the bottom line, of (45) and solve for M_-:

$$1 = |M_-|^2(\lambda^2 + (\omega + \Delta)^2) = |M_-|^2\alpha^2 \Longrightarrow |M_-| = 1/\alpha \tag{48}$$

so we may write

$$\begin{pmatrix} \langle 0|\mu_-\rangle \\ \langle 1|\mu_-\rangle \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = N_+ \begin{pmatrix} -\lambda \\ \omega + \Delta \end{pmatrix} = \begin{pmatrix} -\lambda/\alpha \\ (\omega + \Delta)/\alpha \end{pmatrix} \tag{49}$$

Therefore, we have the normalized eigenvectors (up to an overall phase)

$$\boxed{|\mu_+\rangle = \frac{\omega + \Delta}{\alpha}|0\rangle + \frac{\lambda}{\alpha}|1\rangle \quad \text{and} \quad |\mu_-\rangle = -\frac{\lambda}{\alpha}|0\rangle + \frac{\omega + \Delta}{\alpha}|0\rangle} \tag{50}$$

We can express the normalized eigenvectors as

$$(c_1/\alpha, c_2/\alpha) \quad \text{and} \quad (-c_2/\alpha, c_1.\alpha) \quad \text{for} \quad \boxed{c_1 \equiv \omega + \Delta \quad \text{and} \quad c_2 \equiv \lambda} \tag{51}$$

(b) To reiterate, if a comp problem gives you equations or defines variables that can be used to simplify your answer, use them! In this case, we will use the variables $E_\pm$, c_1, and c_2 from part (a). (Using these variables would also allow you to get partial credit if you weren't able to solve part (a) in time.)

To compute the time evolution of the initial state $|0\rangle$, the first step is to write the initial state in the energy eigenbasis $|\mu_\pm\rangle$, where, by part (a),

$$|\mu_+\rangle = (c_1/\alpha)\,|0\rangle + (c_2/\alpha)\,|1\rangle \quad \text{and} \quad |\mu_-\rangle = -(c_2/\alpha)\,|0\rangle + (c_1/\alpha)\,|1\rangle \tag{52}$$

We can write $|0\rangle$ in terms of $|\mu_\pm\rangle$ using the inner product:

$$\begin{aligned} |0\rangle &= |\mu_+\rangle\,\langle\mu_+|0\rangle + |\mu_-\rangle\,\langle\mu_-|0\rangle \\ &= (c_1/\alpha)\,|\mu_+\rangle - (c_2/\alpha)\,|\mu_-\rangle \end{aligned} \tag{53}$$

Now, we can time-evolve each of the energy eigenstates to get the state at a later time:

$$|\psi(t)\rangle = e^{-iHt/\hbar}\,|0\rangle = (c_1/\alpha)e^{-iE_+t/\hbar}\,|\mu_+\rangle - (c_2/\alpha)e^{-iE_-t/\hbar}\,|\mu_-\rangle \tag{54}$$

To find the probability of finding the system in state $|1\rangle$, take the inner product with that state:

$$\begin{aligned} \langle 1|\psi(t)\rangle &= (c_1/\alpha)e^{-iE_+t/\hbar}\,\langle 1|\mu_+\rangle - (c_2/\alpha)e^{-iE_-t/\hbar}\,\langle 1|\mu_-\rangle \\ &= (c_1/\alpha)e^{-iE_+t/\hbar}(c_2/\alpha) - (c_2/\alpha)e^{-iE_-t/\hbar}(c_1/\alpha) \\ &= \frac{c_1c_2}{\alpha^2}\left(e^{-iE_+t/\hbar} - e^{-iE_-t/\hbar}\right) \end{aligned} \tag{55}$$

From part (a), we have $c_1 = \omega + \Delta$, $c_2 = \lambda$, and $E_\pm = \hbar(\omega \pm \Delta)$. The problem also tells us that $\alpha^2 = 2\Delta(\omega+\Delta)$. Plugging all this in and simplifying, we get

$$\begin{aligned} \langle 1|\psi(t)\rangle &= \frac{(\omega+\Delta)\lambda}{2\Delta(\omega+\Delta)}\left(e^{-i(\omega+\Delta)t} - e^{-i(\omega-\Delta)t}\right) \\ &= e^{-i\omega t}\,\frac{\lambda}{\Delta}\,\frac{e^{-i\Delta t} - e^{i\Delta t}}{2} \\ &= e^{-i\omega t}\,\frac{\lambda}{\Delta}\,(-i\sin(\Delta t)) \quad \text{using } \sin x = \frac{e^{ix} - e^{-ix}}{2i} \end{aligned} \tag{56}$$

The probability of finding the system in state $|1\rangle$ is the square of the absolute value of $\langle 1|\psi(t)\rangle$:

$$P_{0\to 1}(t) = |\langle 1|\psi(t)\rangle|^2 = \boxed{\frac{\lambda^2}{\Delta^2}\sin^2(\Delta t)} \tag{57}$$

which is the answer given by the problem.

(c) This is a time-dependent perturbation theory problem, so here is a quick review of time-dependent perturbation theory (it is the same as the one presented in 2020 Q1):

The key to deriving the formulas for time-dependent perturbation theory is to work in the interaction picture. For an unperturbed, time-independent Hamiltonian H_0 added to a time-dependent perturbation $V(t)$,

$$H(t) = H_0 + V(t) \tag{58}$$

we write the interaction picture by folding the time-evolution of each state under H_0 into the quantum operators. If $\mathcal{O}_S$ is an operator in the (typical) Schrödinger picture, the equivalent operator $\mathcal{O}_I$ in the interaction picture is defined by

$$\mathcal{O}_I(t) \equiv e^{iH_0t/\hbar}\,\mathcal{O}_S\,e^{-iH_0t/\hbar} \tag{59}$$

To make sure that the expectation value $\langle\psi|\mathcal{O}|\psi\rangle$ is the same in both pictures, we must change the state $|\psi\rangle$ accordingly. If $|\psi_S(t)\rangle$ is a time-evolved ket in the Schrödinger picture, the equivalent ket $|\psi_I(t)\rangle$ in the interaction picture is defined by

$$|\psi_I(t)\rangle \equiv e^{iH_0t/\hbar}\,|\psi_S(t)\rangle \tag{60}$$

Kets in the interaction picture obey the Schrödinger equation for the perturbation Hamiltonian $V_I(t)$ in the interaction picture:

$$i\hbar\frac{\partial}{\partial t}\,|\psi_I(t)\rangle = V_I(t)\,|\psi_I(t)\rangle \tag{61}$$

We can integrate this equation (applying the initial condition for the state ψ at a reference time t_0) to get

$$|\psi_I(t)\rangle = |\psi_I(t_0)\rangle - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,V_I(t')\,|\psi_I(t')\rangle \tag{62}$$

To lowest order in perturbation theory, $|\psi_I(t')\rangle \approx |\psi_I(t_0)\rangle$, so this equation becomes

$$|\psi_I(t)\rangle = |\psi_I(t_0)\rangle - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,V_I(t')\,|\psi_I(t_0)\rangle \quad \text{to lowest order} \tag{63}$$

Now suppose that at $t = t_0$, the system is in an eigenstate $|n\rangle$ of H_0, and we are interested in the transition amplitude to another eigenstate $|m\rangle$. We can then take the inner product of (63) with $\langle m|$:

$$\begin{aligned}\langle m|\psi_I(t)\rangle &= \langle m|n\rangle - \frac{i}{\hbar}\int_{t_0}^{t} dt'\;\langle m|V_I(t')|n\rangle \\ &= \delta_{mn} - \frac{i}{\hbar}\int_{t_0}^{t} dt'\,e^{i(E_m-E_n)t'/\hbar}\,\langle m|V_S(t')|n\rangle \quad \text{to lowest order}\end{aligned} \tag{64}$$

In the second line, we have applied the definition of an operator in the interaction picture (59). Since $\langle m|\psi_I(t)\rangle = e^{-iE_mt/\hbar}\,\langle m|\psi_S(t)\rangle$ by (60), this is what we need to calculate transition probabilities.

As always,

For all time-dependent perturbation theory problems, start by calculating the matrix elements of the perturbation Hamiltonian between initial and final states.

In this case, the perturbation Hamiltonian is H_1, and its matrix elements are already given. The initial state is $|0\rangle$, and the final state is $|1\rangle$. Therefore, by (64), we have

$$\langle 1|\psi_I(t)\rangle = -\frac{i}{\hbar}\int_{0}^{t} dt'\,e^{i(E_1-E_0)t'/\hbar}\,\langle 1|H_1|0\rangle \quad \text{to lowest order} \tag{65}$$

Note that E_0 and E_1 are the *unperturbed* energy eigenstates, i.e., those for the Hamiltonian H_0:

$$E_0 = 2\hbar\omega \quad \text{and} \quad E_1 = 0 \quad \text{because} \quad \begin{pmatrix}\langle 0|H_0|0\rangle & \langle 0|H_0|1\rangle \\ \langle 1|H_0|0\rangle & \langle 1|H_0|1\rangle\end{pmatrix} = \begin{pmatrix}2\hbar\omega & 0 \\ 0 & 0\end{pmatrix} \tag{66}$$

Therefore, using the fact that $\langle 1|H_1|0\rangle = \hbar\lambda$ and plugging into (65) we get

$$\begin{aligned}
\langle 1|\psi_I(t)\rangle &= -i\lambda \int_0^t dt'\, e^{2i\omega t'} \\
&= -i\lambda \cdot \frac{1}{2i\omega}\left[e^{2i\omega t'}\right]_0^t \\
&= -\frac{\lambda}{2\omega}\left(e^{2i\omega t} - 1\right) \\
&= -\frac{\lambda}{2\omega} e^{i\omega t}\left(e^{i\omega t} - e^{-i\omega t}\right) \\
&= -i\frac{\lambda}{\omega} e^{i\omega t}\sin(\omega t) \quad \text{to lowest order, using } \sin x = \frac{e^{ix} - e^{-ix}}{2i}
\end{aligned} \tag{67}$$

The probability of finding the system in state $|1\rangle$ is the square of the absolute value of $\langle 1|\psi_I(t)\rangle$, since the Schrödinger picture and the interaction picture differ by an overall phase:

$$P_{0\to 1}(t) = |\,\langle 1|\psi_I(t)\rangle\,|^2 = \boxed{\frac{\lambda^2}{\omega^2}\sin^2(\omega t)} \quad \text{to lowest order} \tag{68}$$

(d) In the limit of $\omega \gg \lambda$, we may expand Δ^2 in a Taylor series:

$$\Delta^2 = \omega^2 + \lambda^2 \approx \omega^2, \quad \text{so} \quad \Delta \approx \omega \quad \text{for } \omega \gg \lambda \tag{69}$$

Then, the part (b) answer becomes

$$P_{0\to 1}(t) = \frac{\lambda^2}{\Delta^2}\sin^2(\Delta t) \approx \boxed{\frac{\lambda^2}{\omega^2}\sin^2(\omega t)} \tag{70}$$

which matches the part (c) answer.