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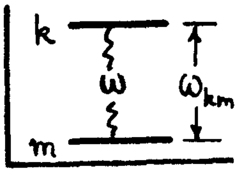
1992 **Φ507 Problems** **Assigned: 4/13. Due: 4/20/92.** Y6 12 ⑫

㊴ [20 pts]. Consider a pulsed harmonic perturbation $V_{ij}(t) = 2\hbar\,\Omega_{ij}\cos\omega t$, applied at $t=0$ to a QM system, in the case where ω approaches an exact resonance for transitions $m \leftrightarrow k$, i.e. $\underline{\underline{\nu = (\omega_{km} - \omega) \to 0}}$. In class, we remarked [NOTES, p. tD6] that the first-order transition amplitude is $a_k^{(1)}(t) \simeq -i\Omega_{km} t$, and hence cannot be correct as $t \to$ large. Here we remedy that situation by solving a new version of the $m \to k$ transition problem very near resonance ($\nu \simeq 0$). We make an exactly solvable two-level problem out of $m \leftrightarrow k$.



(A) When $\nu = (\omega_{km} - \omega) \to 0$, basically only the states m & k participate in transitions, to good approximation. Show then that the "exact" eqtns for the amplitudes are: $\boxed{i\dot{a}_k = \Omega_{km}\,a_m\,e^{i\nu t},\quad i\dot{a}_m = \Omega_{mk}\,a_k\,e^{-i\nu t}}$; the approximation is that all other states are so far off resonance they can be ignored. We have a two-level problem.

(B) The problem in part (A) can be solved exactly (assuming Ω_{km} is independent of t). Find $a_k(t)$, assuming the system was initially in state m: $a_m(0)=1$, $a_k(0)=0$. Define and use the quantity: $Q = [1 + (2|\Omega_{km}|/\nu)^2]^{1/2}$. Also find $a_m(t)$.

(C) Sketch the $m \to k$ transition probability $|a_k|^2$ vs. ν. Now what happens as $\nu \to 0$?

㊵ A QM state of nominal energy E_n which undergoes exponential decay at rate Γ_n is represented by a wavefcn: $\underline{\underline{\psi_n(x,t) = [\phi_n(x)\,e^{-(i/\hbar)E_n t}]\,e^{-\frac{1}{2}\Gamma_n t}}}$; $|\psi_n|^2 = |\phi_n|^2 e^{-\Gamma_n t}$ decays with a "lifetime" $\tau_n = 1/\Gamma_n$. Fourier transform $\psi_n(x,t) \to \tilde{\psi}_n(x,\omega)$ to a frequency variable $\omega = E/\hbar$. Then $|\tilde{\psi}_n(x,E)|^2$ vs. E should give the spectrum of photon energies which can be emitted during the decay. Find and analyse this spectrum. Also, evaluate $\int_{-\infty}^{\infty} |\tilde{\psi}(x,E)|^2 dE$. Why is this "interesting"?

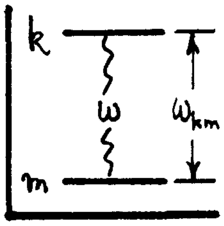
㊶ A QM harmonic oscillator (1D, mass m & spring cnst k) is initially in its ground state, with (normalized) wavefcn: $\underline{\underline{\phi(x) = (\alpha/\pi)^{1/4}\,e^{-\frac{1}{2}\alpha x^2}}}$, w/ $\alpha = \sqrt{km}/\hbar$. The spring cnst is suddenly changed from k to Nk, w/ $N>0$ some numerical factor. Find the probability P_0 that the oscillator will remain in its (new) ground state. Calculate P_0 for $N=2$, and $N=\frac{1}{2}$. Over what range of N-values will P_0 be greater than 50%?

(39) [20 pts]. Pulsed harmonic perturbation: case of exact resonance for $m \rightarrow k$.

(A) 1. From the exact amplitude eqtns in class notes, p. tD3, Eq. (6)...

$$\rightarrow i\hbar\dot{a}_\lambda = \sum_\mu V_{\lambda\mu}(t)\, a_\mu\, e^{i\omega_{\lambda\mu}t}, \quad \text{or}\quad i\dot{a}_\lambda = \sum_\mu \Omega_{\lambda\mu}\, a_\mu \big[\overset{①}{e^{i(\omega_{\lambda\mu}+\omega)t}} + \overset{②}{e^{i(\omega_{\lambda\mu}-\omega)t}}\big]. \qquad (1)$$

If ω is very close to ω_{km}, so that only levels k & m show any strong transition activity, then this ∞ set of eqtns reduces to just two: one for $\lambda = k$ & $\mu = m$, and one for $\lambda = m$ & $\mu = k$. In the first case, term ② has $\omega_{\lambda\mu} = \omega_{km}$ (assumed +ve) and oscillates at $\nu = \omega_{km} - \omega$. Term ① oscillates at a very high frequency $(\nu + 2\omega)$, is non-resonant, and is thus discarded. Eqtn is:



$$\rightarrow i\,\dot{a}_k = \Omega_{km}\, a_m\, e^{i\nu t}, \quad \text{w/}\ \nu = \omega_{km} - \omega. \qquad (2a)$$

In the second case, $\omega_{\lambda\mu} = \omega_{mk} = -\omega_{mk}$, and term ① oscillates at $(-)\nu$. Term ② oscillates at $-(\nu + 2\omega)$, and is discarded because it is non-resonant. Eqtn is:

$$\rightarrow i\,\dot{a}_m = \Omega_{mk}\, a_k\, e^{-i\nu t}. \quad \underline{\text{NOTE}}:\ \Omega_{mk} = \Omega_{km}^*. \qquad (2b)$$

As required, Eqs. (2a) & (2b) together describe $m \leftrightarrow k$ very near resonance, $\nu \simeq 0$.

(B) 2. Decouple Eqs. (2) by taking $\frac{d}{dt} \times$ Eq. (2a), and using (2b) to substitute for $\dot{a}_m$. With a minor bit of algebra, get a 2nd-order ODE for a_k, viz:

$$\Big[\!\Big[\ddot{a}_k - i\nu\dot{a}_k + |\Omega_{km}|^2 a_k = 0.\Big]\!\Big] \qquad (3)$$

Solutions will be of the form: $a_k(t) = e^{\alpha t}$, if α satisfies the secular eqtn:

$$\rightarrow \alpha^2 - i\nu\alpha + |\Omega_{km}|^2 = 0 \Rightarrow \alpha_{1,2} = \frac{i\nu}{2}(1 \pm Q), \quad \text{w/}\ \underline{\underline{Q = \left[1 + \left(\frac{2|\Omega_{km}|}{\nu}\right)^2\right]}}. \qquad (4)$$

General solution for $a_k(t)$ is then (w/ A & B = cnsts):

$$\rightarrow a_k(t) = A\,e^{\alpha_1 t} + B\,e^{\alpha_2 t}. \qquad (5)$$

3. The initial conditions for (5) are: $a_k(0) = 0$, and [use (2a)]: $\dot{a}_k(0) = -i\Omega_{km}$.

So

$$\begin{aligned} A + B &= 0 \\ \alpha_1 A + \alpha_2 B &= -i\Omega_{km} \end{aligned} \Rightarrow A = -\frac{\Omega_{km}}{\nu Q}, \quad B = -A = \frac{\Omega_{km}}{\nu Q} \qquad (6)$$

Put A & B of (6) into (5) to obtain the desired k-state "exact" amplitude

$$\boxed{a_k(t) = \left(\frac{2\Omega_{km}}{i\nu Q}\right) e^{\frac{1}{2}i\nu t} \sin\left(\tfrac{1}{2}Q\nu t\right)}. \qquad \underset{\sim\sim}{(7)}$$

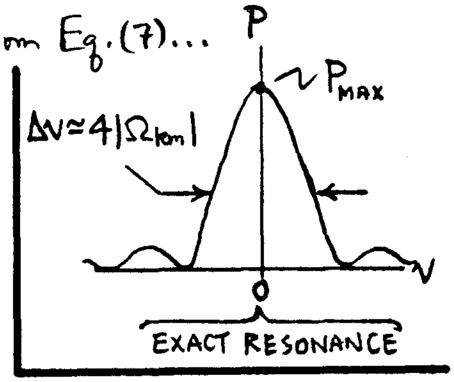
The m-state amplitude can be derived from a_k via: $a_m = i\dot{a}_k/\Omega_{km}e^{i\nu t}$, per Eq. (2a). For future reference: $\underline{\underline{a_m(t) = e^{-\frac{1}{2}i\nu t}\left[\cos\left(\tfrac{1}{2}Q\nu t\right) - \tfrac{i}{Q}\sin\left(\tfrac{1}{2}Q\nu t\right)\right]}}$. $\underset{\sim\sim}{(8)}$

These amplitudes (Eqs. (7) & (8)) satisfy the stated conditions: $a_k(0) = 0$, $a_m(0) = 1$.

(C)

$\underline{\underline{4.}}$ The m→k transition probability is $|a_k|^2$, or -- from Eq. (7)...

$$\left[\begin{array}{l} P(m\to k) = |a_k(t)|^2 = |\Omega_{km}|^2\left(\dfrac{\sin^2\tilde{\nu}t}{\tilde{\nu}^2}\right), \qquad \underset{\sim\sim}{(9)} \\ \text{w/}\ \tilde{\nu} = \dfrac{Q\nu}{2} = \left[(\nu/2)^2 + |\Omega_{km}|^2\right]^{1/2}, \quad \nu = \omega_{km} - \omega. \end{array}\right.$$



$P(m\to k)$ vs. ν specifies the spectral lineshape for the m→k transition. Now, at exact resonance, $\nu = 0$ and $\tilde{\nu} = |\Omega_{km}|$, so that

$$\underline{\underline{P(m\to k)\big|_{MAX} = \sin^2(|\Omega_{km}|t)}}, \text{ at exact resonance } (\nu = 0). \qquad \underset{\sim\sim}{(10)}$$

First-order theory predicted $P(m\to k)|_{max} = (|\Omega_{km}|t)^2$, which is just the first term in the Taylor series for $\sin^2(|\Omega_{km}|t)$. Now we have a <u>bounded</u> variation for $P(m\to k)_{MAX}$... it just oscillates between 1 (full occupation) and 0 (quantum oscillation back to m) at the frequency $|\Omega_{km}|$, which is determined by the <u>strength</u> of the perturbation V, <u>not</u> its frequency.

$\underline{\underline{5.}}$ The <u>width</u> of $P(m\to k)$ in above sketch is also determined by the coupling matrix element $|\Omega_{km}|$. The half power points for $P(m\to k)$ of (9) are at...

$$\to |\Omega_{km}|^2/\tilde{\nu}^2 = \tfrac{1}{2} \Rightarrow \left(\tfrac{\nu}{2}\right)^2 = |\Omega_{km}|^2, \text{ w/ } \nu = \pm 2|\Omega_{km}|. \qquad \underset{\sim\sim}{(11)}$$

So the FWHM is $\Delta\nu = 4|\Omega_{km}|$. By supplying too much power (i.e. making the amplitude of V too large), the m→k lineshape can be excessively broadened.

㊵ Find the energy spectrum of the decaying state: $\Psi_n = [\phi_n e^{-(i/\hbar)E_n t}]\, e^{-\frac{1}{2}\Gamma_n t}$.

1. Ψ_n is of course defined (only) @ $t \geqslant 0$. ¶ Its spectral decomposition is:

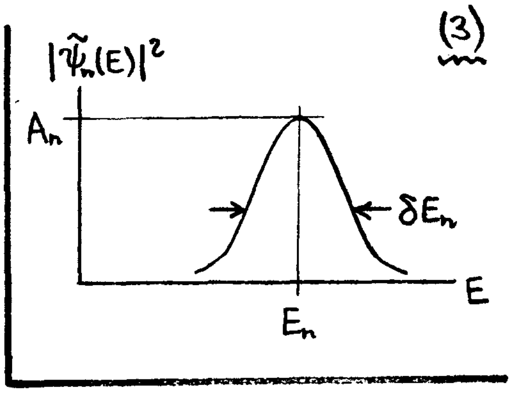
$$\left[\begin{array}{l} \Psi_n(x,t) = \int_{-\infty}^{\infty} \tilde{\Psi}_n(x,E)\, e^{-(i/\hbar)Et}\, dE, \quad \text{w/ usual Fourier frequency } \omega = \frac{E}{\hbar}; \\ \text{so} \quad \tilde{\Psi}_n(x,E) = \frac{1}{2\pi\hbar}\int_0^{\infty} \Psi_n(x,t)\, e^{+(i/\hbar)Et}\, dt. \end{array}\right. \qquad (1)$$

$|\tilde{\Psi}_n(x,E)|^2$ vs. E gives the energy spectrum (lineshape) for the decay. Since x is just a spectator variable, then -- for the given Ψ_n...

$$\rightarrow \tilde{\Psi}_n(E) = \frac{\phi_n}{2\pi\hbar}\int_0^{\infty} e^{-G_n t}\, dt, \quad G_n = \tfrac{1}{2}\Gamma_n + \tfrac{i}{\hbar}(E_n - E). \qquad (2)$$

This integral is convergent for $\Gamma_n > 0$: $\int_0^{\infty} e^{-G_n t}\, dt = 1/G_n$. Then...

$$\underline{\underline{\tilde{\Psi}_n(E) = \frac{\phi_n}{2\pi\hbar} \Big/ \frac{\Gamma_n}{2}\left[1 + i\left(\frac{E_n - E}{\hbar\Gamma_n/2}\right)\right]}}. \qquad (3)$$



2. The lineshape is $|\tilde{\Psi}_n(E)|^2$. From Eq. (3):

$$\boxed{|\tilde{\Psi}_n(E)|^2 = A_n \Big/ \left[1 + \left(\frac{E - E_n}{\hbar\Gamma_n/2}\right)^2\right]},$$

$$\text{w/ } A_n = |\phi_n/\pi\hbar\Gamma_n|^2. \qquad (4)$$

The decay lineshape is a Lorentzian, centered at $E = E_n$, of max. amplitude A_n, and width (FWHM) $\underline{\underline{\delta E_n = \hbar\Gamma_n}}$. E_n is the most probable of the observable decay photon energies. But -- in accord with the uncertainty principle ($\delta E_n \delta t \sim \hbar$), we will see energies spread over $E_n \pm \delta E_n$.

3. The area under the lineshape in (4) is:

$$\longrightarrow \int_{-\infty}^{\infty} |\tilde{\Psi}_n(E)|^2 dE = |\phi_n/\pi\hbar\Gamma_n|^2 \cdot \frac{\hbar\Gamma_n}{2}\int_{-\infty}^{\infty}\frac{dx}{1+x^2} = \underline{\underline{|\phi_n|^2/2\pi\hbar\Gamma_n}}. \qquad (5)$$

This area is independent of the decay energy E_n. It is universally true of all exponential decays. As well, all such decays generate a Lorentzian line, per (4).

= ¶ Picture is: Ψ_n is prepared (excited) at $t = 0$. Thereafter, it decays exponentially.

㊶ Analyse QM SHO for sudden changes in spring cnst k.

1. The initial and final states are assumed to be the ground states...

$$\left[\begin{array}{l} \phi(x) = (\alpha/\pi)^{1/4}\, e^{-\frac{1}{2}\alpha x^2}, \quad \tilde{\Phi}(x) = (\tilde{\alpha}/\pi)^{1/4}\, e^{-\frac{1}{2}\tilde{\alpha} x^2} \\ \text{where: } \alpha = \sqrt{km}/\hbar, \quad \tilde{\alpha} = \sqrt{N}\,\alpha \quad (\text{since } \tilde{k} = Nk). \end{array}\right\} \quad (1)$$

If the $k \rightarrow \tilde{k}$ change is "sudden" (taking place over time Δt which is short compared to the natural oscillator period $\tau = 2\pi/\sqrt{k/m}$), then the probability of $\phi \rightarrow \tilde{\Phi}$ is just $P_0 = |\langle\tilde{\Phi}|\phi\rangle|^2$, where the overlap is...

$$\langle\tilde{\Phi}|\phi\rangle = \left(\frac{\alpha}{\pi}\right)^{1/4}\left(\frac{\tilde{\alpha}}{\pi}\right)^{1/4}\int_{-\infty}^{\infty} e^{-\frac{1}{2}(\alpha+\tilde{\alpha})x^2}\,dx = \sqrt{2}\,(\alpha\tilde{\alpha})^{1/4}/\sqrt{\alpha+\tilde{\alpha}}$$

$$\text{or } \langle\tilde{\Phi}|\phi\rangle = \left[4\alpha\tilde{\alpha}/(\alpha+\tilde{\alpha})^2\right]^{1/4} = \left[4\sqrt{N}/(1+\sqrt{N})^2\right]^{\frac{1}{4}}; \quad (2)$$

$$\text{so } \boxed{P_0(N) = 2N^{1/4}/(1+\sqrt{N})} \quad (3)$$

probability for SHO to remain in ground state when $k \rightarrow Nk$.

The fact that $P_0(1) = 1$ verifies the normalisation of ϕ in Eq. (1).

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2. From (3): $P_0(N=2) = 0.9852$, and $P_0(N=\frac{1}{2}) = 0.9852$ also.* $P_0(N) > \frac{1}{2}$ over a range in N such that

$$\text{for } x = N^{1/4}: \quad \frac{2x}{1+x^2} > \frac{1}{2} \Rightarrow x^2 - 4x + 1 < 0,$$

$$\text{or } (2-\sqrt{3}) < x < (2+\sqrt{3}), \quad \text{and } \underline{\underline{\frac{1}{194} < N < 194}}. \quad (4)$$

Evidently it requires a *big* change in k to get the SHO out of its ground state. The ground state is "stable" by this criterion.

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* In Eq. (3), we have the symmetry: $P_0(1/N) = P_0(N)$.