Physics 512 **Winter 2003**

Homework Set #9 – Solutions

Note: The homework set posted on the web had a second page (part c) of problem #3 and problem #4). I mistakenly omitted the second page on the set I handed out in class, so only the first three problems are required. What should have been problem #4 is now part of Homework #10.

1. We consider first order time dependent perturbation theory for a Hamiltonian $H(t) = H_0 + V(t)$. Suppose that a system is initially in an eigenstate $|s\rangle$ of H_0 at time t_0. Let $\mathcal{O}$ be some observable of the system. Show that the expectation value of $\mathcal{O}$ at time t is given to first order in $V(t)$ by

$$\langle\psi(t)|\mathcal{O}|\psi(t)\rangle = \langle s|\mathcal{O}|s\rangle - \frac{i}{\hbar}\int_{t_0}^{t}\langle s|[\widetilde{\mathcal{O}}(t), \widetilde{V}(t')]|s\rangle\, dt'$$

where $\widetilde{\mathcal{O}}(t)$ and $\widetilde{V}(t)$ are in the interaction picture.

Since we are interested in a system at a later time t, we transform to the interaction picture and use the time evolution operator. Going from the Schrödinger picture to the interaction picture is simple (we just put tilde's over everything)

$$\langle\psi(t)|\mathcal{O}|\psi(t)\rangle = \langle\widetilde{\psi}(t)|\widetilde{\mathcal{O}}(t)|\widetilde{\psi}(t)\rangle$$

To first order, the time evolution operator in the interaction picture gives

$$|\widetilde{\psi}(t)\rangle = \widetilde{T}(t, t_0)|\widetilde{s}\,\rangle = \left[1 - \frac{i}{\hbar}\int_{t_0}^{t}\widetilde{V}(t')\, dt'\right]|\widetilde{s}\,\rangle$$

where $|\widetilde{s}\rangle$ is the initial state, converted to the interaction picture. Since we assume that V is Hermitian (so that $\tilde{V}$ is also Hermitian), the bra state evolves similarly

$$\langle\widetilde{\psi}(t)| = \langle\widetilde{s}\,|\left[1 + \frac{i}{\hbar}\int_{t_0}^{t}\widetilde{V}(t')\, dt'\right]$$

We may combine these expressions to obtain

$$\begin{aligned}\langle\psi(t)|\mathcal{O}|\psi(t)\rangle &= \langle\widetilde{s}\,|\left[1 + \frac{i}{\hbar}\int_{t_0}^{t}\widetilde{V}(t')\, dt'\right]\widetilde{\mathcal{O}}(t)\left[1 - \frac{i}{\hbar}\int_{t_0}^{t}\widetilde{V}(t')\, dt'\right]|\widetilde{s}\,\rangle \\ &= \langle\widetilde{s}\,|\widetilde{\mathcal{O}}(t)|\widetilde{s}\,\rangle + \frac{i}{\hbar}\int_{t_0}^{t}\Big(\langle\widetilde{s}\,|\widetilde{V}(t')\widetilde{\mathcal{O}}(t)|\widetilde{s}\,\rangle - \langle\widetilde{s}\,|\widetilde{\mathcal{O}}(t)\widetilde{V}(t')|\widetilde{s}\,\rangle\Big)\, dt' \\ &= \langle s|\mathcal{O}|s\rangle - \frac{i}{\hbar}\int_{t_0}^{t}\langle\widetilde{s}\,|[\widetilde{\mathcal{O}}(t)\widetilde{V}(t')]|\widetilde{s}\,\rangle\, dt'\end{aligned}$$

(where we have ignored the higher order term where $\widetilde{V}$ appears twice). Note that in the first term we have converted back to the Schrödinger picture by removing the tilde's. Finally, since $|s\rangle$ is an eigenstate of H_0, it is easily converted into the interaction picture (at time t_0) according to

$$|\widetilde{s}\,\rangle = e^{iH_0t_0/\hbar}|s\rangle = e^{iE_st_0/\hbar}|s\rangle$$

Since this is just a phase relating $|s\rangle$ to $\widetilde{s}\,\rangle$, it cancels from the bra-ket $\langle\widetilde{s}\,|\cdots|\widetilde{s}\,\rangle$. This proves the result

$$\langle\psi(t)|\mathcal{O}|\psi(t)\rangle = \langle s|\mathcal{O}|s\rangle - \frac{i}{\hbar}\int_{t_0}^{t}\langle s|[\widetilde{\mathcal{O}}(t),\widetilde{V}(t')]|s\rangle\,dt'$$

2. Apply first-order time dependent perturbation theory to a forced harmonic oscillator

$$H = (a^\dagger a + \tfrac{1}{2})\hbar\omega + f(t)a + f^*(t)a^\dagger$$

which is initially in the ground state, and compare the transition probability with the exact result

$$P_{n\leftarrow 0} = \frac{1}{n!}\left|\frac{g(\omega)}{\hbar}\right|^{2n} e^{-|g(\omega)/\hbar|^2}$$

where

$$g(\omega) = \int_{-\infty}^{\infty} e^{-i\omega t'} f(t')\,dt'$$

is the Fourier transform of the generalized force $f(t)$. Calculate the energy transfer to the oscillator exactly and also in perturbation theory. Show that the energies agree, even though the probabilities do not (see Exercise 19.2).

We take the time-dependent perturbation to be

$$V(r) = f(t)a + f^*(t)a^\dagger$$

Then first-order time dependent perturbation theory gives a transition amplitude

$$\begin{aligned}\mathcal{A}_{n\leftarrow 0} &= -\frac{i}{\hbar}\int_{-\infty}^{\infty} e^{i\omega_{n0}t'}\langle n|V(t')|0\rangle\,dt' \\ &= -\frac{i}{\hbar}\int_{-\infty}^{\infty} e^{in\omega t'}\langle n|(f(t')a + f^*(t')a^\dagger)|0\rangle\,dt'\end{aligned}$$

(where we have extended the time limits from the infinite past to the infinite future). Since $a|0\rangle = 0$ and $a^\dagger|0\rangle = |1\rangle$, we find

$$\begin{aligned}\mathcal{A}_{n\leftarrow 0} &= -\frac{i}{\hbar}\langle n|1\rangle\int_{-\infty}^{\infty} e^{in\omega t'} f^*(t')\,dt' \\ &= -\frac{i}{\hbar}\delta_{n,1}\int_{-\infty}^{\infty} e^{i\omega t'} f^*(t')\,dt' = -\frac{i}{\hbar}g^*(\omega)\delta_{n,1}\end{aligned}$$

The transition probability is thus

$$P_{1\leftarrow 0} = |\mathcal{A}_{1\leftarrow 0}|^2 = \left|\frac{g(\omega)}{\hbar}\right|^2$$

and is only non-vanishing for transitions to the first excited state of the harmonic oscillator. This is in contrast to the exact result, which has non-zero probability to end up in any excited state. This discrepancy arises because for each order in perturbation theory the potential can only act once. With $V(t)$ linear in creation and annihilation operators, we would need to go to n-th order perturbation theory to find a transition probability to the n-th state. This is apparent from the exact result, where the leading behavior gives $P_{n\leftarrow 0} \sim |g(\omega)|^{2n}$ (so that the amplitude must be related to $g(\omega)^n$, which in turn corresponds to n powers of the perturbation).

The energy transfer to the oscillator is given by

$$\Delta E = \sum_{n=1}^{\infty} P_{n\leftarrow 0}(E_n - E_0) = \hbar\omega \sum_{n=1}^{\infty} n\, P_{n\leftarrow 0}$$

For the perturbation result, this gives simply

$$\Delta E_{\text{pert}} = \hbar\omega \left|\frac{g(\omega)}{\hbar}\right|^2$$

On the other hand, for the exact probabilities, we have to sum over all states

$$\begin{aligned}\Delta E_{\text{exact}} &= \hbar\omega \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left|\frac{g(\omega)}{\hbar}\right|^{2n} e^{-|g(\omega)/\hbar|^2} \\ &= \hbar\omega \left|\frac{g(\omega)}{\hbar}\right|^2 e^{-|g(\omega)/\hbar|^2} \sum_{n=1}^{\infty} \frac{1}{(n-1)!} \left|\frac{g(\omega)}{\hbar}\right|^{2(n-1)}\end{aligned}$$

By shifting n in the sum, we see that it is just the Taylor series for the exponential $e^{|g(\omega)/\hbar|^2}$. Hence the exponentials cancel, and we find

$$\Delta E_{\text{exact}} = \hbar\omega \left|\frac{g(\omega)}{\hbar}\right|^2$$

so that both the perturbation theory and the exact results agree with each other. Since the exact energy transfer is only quadratic in $g(\omega)$, this can only be generated at first order in the perturbative expansion (each higher order gives more $g(\omega)$'s). This indicates, at least after knowing the full answer, that the first order result must be exact. We have already seen this effect in the earlier homework problem on a time independent perturbation of the harmonic oscillator by a constant force.

3. This is similar to Sakurai, Chapter 5, Problem 25. The unperturbed Hamiltonian of a two-state system is represented by

$$H_0 = \begin{pmatrix} E_1^0 & 0 \\ 0 & E_2^0 \end{pmatrix}$$

There is, in addition, a time-dependent perturbation

$$V(t) = \lambda \begin{pmatrix} 0 & e^{i\omega t} \\ e^{-i\omega t} & 0 \end{pmatrix} \qquad (\lambda \text{ real })$$

a) At $t = 0$ the system is known to be in the first state, represented by $\binom{1}{0}$. Using time-dependent perturbation theory and assuming that $E_1^0 - E_2^0$ is not close to $\pm\hbar\omega$, derive an expression for the probability for the system to be found in the second state represented by $\binom{0}{1}$ as a function of t (for $t > 0$).

Let us denote the first state $\binom{1}{0}$ *by* $|1\rangle$ *and the second state* $\binom{0}{1}$ *by* $|2\rangle$*. Then the transition amplitude is given by*

$$A_{2\leftarrow 1} = -\frac{i}{\hbar}\int_0^t e^{i\omega_{21}t'}\langle 2|V(t')|1\rangle\, dt'$$

where $\omega_{21} = (E_2^0 - E_1^0)/\hbar$ *and* $\langle 2|V(t')|1\rangle = \lambda e^{-i\omega t'}$*. Then*

$$\begin{aligned} A_{2\leftarrow 1} &= -\frac{i}{\hbar}\int_0^t e^{i\omega_{21}t'}\lambda e^{-i\omega t'}\, dt' = -\frac{i\lambda}{\hbar}\int_0^t e^{i(\omega_{21}-\omega)t'}\, dt' \\ &= -\frac{\lambda}{\hbar}\frac{e^{i(\omega_{21}-\omega)t} - 1}{\omega_{21} - \omega} \\ &= -\frac{2\lambda}{\hbar}e^{i(\omega_{21}-\omega)t/2}\frac{\sin[(\omega_{21} - \omega)t/2]}{\omega_{21} - \omega} \end{aligned}$$

We square this to get the probability

$$P_{2\leftarrow 1} = |A_{2\leftarrow 1}|^2 = \frac{4\lambda^2}{\hbar^2}\frac{\sin^2[(\omega_{21} - \omega)t/2]}{(\omega_{21} - \omega)^2} \tag{1}$$

b) Why is this procedure not valid when $E_1^0 - E_2^0$ is close to $\pm\hbar\omega$?

When $E_1^0 - E_2^0$ *is near* $-\hbar\omega$*, the denominator nearly vanishes, and we can no longer trust the perturbation expansion (which assumed all quantities were "small"). Of course, the corresponding numerator vanishes whenever the denominator does. So the answer may not be obviously wrong. This is in fact the basis for deriving Fermi's Golden rule. While the problem asks for* $E_1^0 - E_2^0$ *close to* $\pm\hbar\omega$*, the transition* $P_{2\leftarrow 1}$ *only breaks down for energy difference* $-\hbar\omega$*. However, one can show that the opposite transition* $P_{1\leftarrow 2}$ *would involve the other denominator, and hence would have trouble around* $+\hbar\omega$*.*

The relative simplicity of this answer, (1), arises because of the harmonic nature of the potential ($e^{i\omega t}$ behavior). Since the time dependence of wavefunctions is given by $\psi(t) \sim e^{-iEt/\hbar}\psi(0)$, is is natural to see that harmonic perturbations (which have the same time dependence behavior) would cause a change in energy of $\pm\hbar\omega$.

c) This system may be solved exactly, since it corresponds to a magnetic resonance Hamiltonian. Find the exact transition probability, and compare with the answer to part *a*).

Note: *This part was omitted on the homework handout (and will not be graded). However it is still interesting, and you may want to have a look*

Let us first recall the magnetic resonance result. The magnetic resonance Hamiltonian was given at the beginning of the semester as

$$H = -\vec{\mu} \cdot \vec{B} = \frac{\hbar}{2}(\omega_0 \sigma_z + \omega_1(\sigma_x \cos\omega t + \sigma_y \sin\omega t)) \tag{2}$$

where the magnetic field has a constant component in the $\hat{z}$ direction (specified by ω_0) and a rotating one in the x-y plane (specified by ω_1). In matrix notation, the Hamiltonian has the form

$$H = \frac{\hbar}{2}\left[\omega_0 \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} + \omega_1 \begin{pmatrix} 0 & e^{-i\omega t} \\ e^{i\omega t} & 0 \end{pmatrix}\right]$$

which is very much like that for the two-state system we have here. Since the transition probability should only depend on the difference in energies, $E_1^0 - E_2^0$, we may associate the magnetic resonance parameters ω_0 and ω_1 with the parameters we have here according to

$$\omega_0 = \frac{(E_1^0 - E_2^0)}{\hbar} \equiv -\omega_{21}, \qquad \omega_1 = \frac{2\lambda}{\hbar} \tag{3}$$

In addition, we must take $\omega \to -\omega$ to agree with the potential $V(t)$.

For the magnetic resonance problem (2), we derived a transition probability

$$P_{|\downarrow\rangle \leftarrow |\uparrow\rangle}(t) = \frac{\omega_1^2}{\Omega^2}\sin^2\frac{\Omega t}{2}, \qquad \Omega = \sqrt{(\omega_0 - \omega)^2 + \omega_1^2}$$

Substituting in the quantities (3), we find the exact probability

$$P_{2\leftarrow 1} = \frac{4\lambda^2}{\hbar^2}\frac{\sin^2[\sqrt{(\omega_{21} - \omega)^2 + 4\lambda^2/\hbar^2}\, t/2]}{(\omega_{21} - \omega)^2 + 4\lambda^2/\hbar^2}$$

which is similar to the perturbative result, (1), except that the denominator no longer blows up on resonance, because of the additional factor $4\lambda^2/\hbar^2$.