PHY662, Spring 2004, Mar. 30, 2004

30th March 2004

1 Miscellaneous

1. Reading: Continue Shankar Ch. 18 for time-dependent perturbation theory, Griffiths Ch. 9.
2. Time-dependent perturbation theory, especially periodic perturbations.

2 Periodic perturbations

REMINDER: We are solving for the time dependence of $\psi(t)$, with $i\hbar\frac{\partial}{\partial t}\psi(t) = H\psi(t)$, where $H(t) = H^0 + H'(t)$.

Our approach generally *will* be to compute transition amplitudes between the unperturbed eigenstates, where the unperturbed eigenstates $|n\rangle$ are the eigenvectors of H^0.

By expanding $|\psi(t)\rangle = \sum_n c_n(t)|n\rangle$ and changing to the coefficients $d_n(t) = c_n(t)e^{iE_n t/\hbar}$, we derived the first order result

$$d_f = \delta_{fi} - \frac{i}{\hbar}\int_0^t dt' \, \langle f|H'|i\rangle e^{i\omega_{fi}t} \, .$$

This formula approximates the amplitude for $\psi(t)$ to be in the state $|f\rangle$, which is an eigentstate of H^0.

Let us consider the specific case

$$H'(t) = \left\{ \begin{array}{cc} 0 & t < 0 \\ V(\vec{r})\cos(\omega t) & t \geq 0 \end{array} \right. .$$

This is a useful arrangement that allows us to cleanly consider the initial eigenstates for $t < 0$ and the effect of adding an oscillating term to the Hamiltonian at later times. Usuallly, the perturbation is present at *all* times, but the state is considered in an eigenstate of H^0 at time $t = 0$. (An alternative derivation to obtain essentially the same results has the perturbation turned on slowly.)

In any case, for this $H'(t)$, we can compute the first-order transition amplitudes to an arbitrary final state $|f\rangle \neq |i\rangle$:

$$\begin{aligned}
d_f &= -\frac{i}{\hbar}\int_0^t dt'\,\langle f|V(\vec{r})|i\rangle \left[\frac{e^{i(\omega+\omega_{fi})t}+e^{i(-\omega+\omega_{fi})t}}{2}\right] \\
&= -\frac{i\langle f|V(\vec{r})|i\rangle}{2\hbar}\left[\frac{e^{i(\omega+\omega_{fi})t}-1}{\omega+\omega_{fi}}+\frac{e^{i(-\omega+\omega_{fi})t}}{\omega_{fi}-\omega}\right] \\
&= \hbar^{-1}\langle f|V(\vec{r})|i\rangle \left[e^{i(\omega+\omega_{fi})t/2}\frac{e^{i(\omega+\omega_{fi})t/2}-e^{-i(\omega+\omega_{fi})t/2}}{2i(\omega+\omega_{fi})}\right. \\
&\quad \left. + \, e^{i(\omega-\omega_{fi})t/2}\frac{e^{i(\omega-\omega_{fi})t/2}-e^{-i(\omega-\omega_{fi})t/2}}{2i(\omega-\omega_{fi})}\right] \\
&= \hbar^{-1}\langle f|V(\vec{r})|i\rangle \left\{e^{i(\omega+\omega_{fi})t/2}\frac{\sin[(\omega+\omega_{fi})t/2]}{\omega+\omega_{fi}}+e^{i(\omega-\omega_{fi})t/2}\frac{\sin[(\omega-\omega_{fi})t/2]}{\omega-\omega_{fi}}\right\}.
\end{aligned}$$

This amplitude can then be used to compute the probability of being in $|f\rangle$ at time t:

$$|d_f|^2 = \frac{|\langle f|V(\vec{r})|i\rangle|^2}{\hbar^2}\left\{\frac{\sin^2[(\omega+\omega_{fi})t/2]}{(\omega+\omega_{fi})^2}+\frac{\sin^2[(\omega-\omega_{fi})t/2]}{(\omega-\omega_{fi})^2}+(\text{crossterm})\right\}.$$

The simplest thing to do at this point is to assume that we are looking at cases where ω_{fi} is near ω. Then, the second term dominates and we get

$$|d_f|^2 \approx \frac{|\langle f|V(\vec{r})|i\rangle|^2}{\hbar^2}\left\{\frac{\sin^2[(\omega-\omega_{fi})t/2]}{(\omega-\omega_{fi})^2}\right\}.$$

Note that the transition probability is oscillatory in time! This can be viewed as an artifact of turning on the potential suddenly. We can also "smooth" out this oscillation by making standard assumptions, which we will do soon. This form is somewhat familiar, though, as it should remind us of the oscillations seen in the probabilities in the problem of magnetic resonance.

3 Averaging to smooth: Fermi's golden rule

The expression for $|d_f|^2$ is put into a standard transition rate expression taking t to be large and by either:

1. Taking a smooth distribution of final states. Example: an electron in an atom being excited by an oscillating field from a bound (discrete) state to an unbound state - the unbound states have a continuum distribution as the wave vectors $\vec{k}$ in free space are smoothly distributed.
2. Taking a smooth *incoherent* mixture of perturbing frequencies. Example: an electron in an atom making a transition from one bound state to another, stimulated by a range of frequencies, simultaneously. Here, the states are discrete, but we average over ω.

For example, let's compute the transition rate from one discrete state to another, but taking a perturbation $H' = \int d\omega\, \rho(\omega) V(\vec{r},\omega) e^{i\omega t}$, where the spectrum of the perturbation is $\rho(\omega)$. The assumption is that the perturbations are *incoherent*, so that there is no interference between the stimulating frequencies and the total transition probability is simply given by an integral over ω:

$$|d_f|^2 \quad \approx \quad \int d\omega\, \rho(\omega) \frac{|\langle f|V(\vec{r},\omega)|i\rangle|^2}{\hbar^2} \left\{ \frac{\sin^2[(\omega-\omega_{fi})t/2]}{(\omega-\omega_{fi})^2} + \frac{\sin^2[(\omega+\omega_{fi})t/2]}{(\omega+\omega_{fi})^2} \right\} .$$

The first expression in curly brackets becomes sharply peaked at $\omega - \omega_{fi} = 0$ as t becomes large, with width $\Delta\omega \approx \frac{2\pi}{t}$ and with total area $\frac{\pi t}{2}$. So we can approximate this function by a delta-function multiplied by the area or weight:

$$\left\{ \frac{\sin^2[(\omega-\omega_{fi})t/2]}{(\omega-\omega_{fi})^2} \right\} \rightarrow \frac{\pi t}{2} \delta(\omega - \omega_{fi}) .$$

This gives the result for the first term:

$$|d_f|^2 \approx \frac{\pi}{2\hbar^2} |\langle f|V(\vec{r},\omega_{fi})|i\rangle|^2 \rho(\omega_{fi}) t .$$

Adding back in the second term, this gives the transition *rate* from $i \rightarrow f$ is (for a $\cos(\omega t)$ perturbation)

$$\Gamma \approx \frac{\pi}{2\hbar^2} |\langle f|V(\vec{r},\omega_{fi})|i\rangle|^2 [\rho(\omega_{fi}) + \rho(-\omega_{fi})] .$$

Another way this is written is

$$\Gamma \approx \frac{2\pi}{\hbar} |\langle f|V(\vec{r},\omega)|i\rangle|^2 \delta(E_f - E_i - \hbar\omega) .$$

In this form, the δ-function has been pulled out for convolving with $\rho(\omega)$ and the perturbation is taken to be of the form $V(\vec{r},\omega)e^{-i\omega t}$.

These formulas are expressions of **Fermi's golden rule**. It is an extremely useful result, under the conditions of a small oscillatory perturbation over a long duration and a continuum in the perturbing frequencies.