Ph195c notes for 4/15/02

Please also have a look at Parsa's writeup on the Forced Harmonic Oscillator.

Time-dependent perturbation theory

Say we have a time-dependent Hamiltonian

$$H(t) = H_0 + \lambda W(t).$$

There will not generally be stationary states for the corresponding Schrödinger Equation, because of the explicit time-dependence. To solve something like an initial-value problem then, we must resort to actual integration of the S.E. since the usual trick of decomposition into energy eigenstates and multiplication by oscillating phase factors does not apply. In principle, $H(t)$ still admits a time-development operator

$$\begin{aligned} i\hbar \frac{d}{dt}|\Psi\rangle &= H(t)|\Psi\rangle, \\ |\Psi(t)\rangle &= \exp\left(\frac{-i}{\hbar}\int_{t_0}^{t} dt' \, H(t')\right)|\Psi(t_0)\rangle \\ &\equiv T(t,t_0)|\Psi(t_0)\rangle, \end{aligned}$$

but obtaining an explicit form for $T(t,t_0)$ can be arbitrarily difficult because of the explicit time-dependence of $W(t)$. So in general we need approximation methods.

Under the assumptions $\lambda \ll 1$ and $H_0 \sim W(t)$, we may be able to use perturbation theory. The spirit of time-dependent perturbation theory is to consider $\lambda W(t)$ as a weak "driving" term that induces transitions among the eigenstates of H_0 – recall that since $W(t)$ is time-dependent there (usually) isn't really a sense in which we could think about leading-order *corrections* to the eigenspectrum. (One exception to this is when $W(t)$ is strictly periodic in time, in which case it is sometimes possible to define quasi-stationary states called Floquet states. These are something like time-domain versions of the Bloch states for a spatially-periodic potential...) Hence our approach will be to derive approximate expressions for transition probabilities such as

$$\begin{aligned} P_{k\leftarrow s}(t) &= |\langle k|\Psi(t)\rangle|^2, \qquad |\Psi(t_0)\rangle = |s\rangle, \\ &= |\langle k|T(t,t_0)|s\rangle|^2, \end{aligned}$$

where $|k\rangle$ and $|s\rangle$ are eigenstates of H_0, the system is initially prepared in state $|s\rangle$ at time t_0, and we are interested in the probability that the perturbation has "kicked" the system into state $|k\rangle$ at (by?) some later time t.

Perturbation expansion in the Interaction Picture

Suppose that the eigenvalues and eigenstates of H_0 are known,

$$H_0|k\rangle = E_k|k\rangle.$$

Then if we work in this basis H_0 is diagonal, and it is easy to compute operator exponentials such as

$$\begin{aligned} T_0(t,t_0) &= \exp\left(\frac{-i}{\hbar}\int_{t_0}^{t} dt'\, H_0\right) \\ &= \exp\left(\frac{-i}{\hbar}H_0(t-t_0)\right). \end{aligned}$$

The *Interaction Picture* is defined by the general change of basis

$$|\Psi(t)\rangle \mapsto \left|\tilde{\Psi}(t)\right\rangle \equiv T_0^{-1}(t,t_0)|\Psi(t)\rangle,$$

$$O \mapsto \tilde{O} \equiv T_0^{-1}(t,t_0)\,O\,T_0(t,t_0).$$

(We have already seen an example of this in the guise of a “rotating frame” for the Bloch Equations.) Note that this change of basis preserves all operator moments,

$$\begin{aligned} \langle O^m\rangle_t &= \langle\Psi(t)|O^m|\Psi(t)\rangle \\ &= \langle\Psi(t)|T_0(t,t_0)T_0^{-1}(t,t_0)\,O^m\,T_0(t,t_0)T_0^{-1}(t,t_0)|\Psi(t)\rangle \\ &= \left\langle\tilde{\Psi}(t)|\tilde{O}^m|\tilde{\Psi}(t)\right\rangle. \end{aligned}$$

In a sense, time evolution associated with H_0 is “taken off” the states and wrapped around the operators instead. Note that this holds even if $[H_0, W(t)] \neq 0$.

The Schrödinger Equation in the Interaction Picture may be derived as follows:

$$\begin{aligned} i\hbar\frac{d}{dt}|\Psi(t)\rangle &= H(t)|\Psi(t)\rangle, \\ i\hbar\frac{d}{dt}\left(T_0(t,t_0)\left|\tilde{\Psi}(t)\right\rangle\right) &= H(t)\,T_0(t,t_0)\left|\tilde{\Psi}(t)\right\rangle, \\ i\hbar\left[\frac{-i}{\hbar}H_0T_0(t,t_0)\left|\tilde{\Psi}(t)\right\rangle + T_0(t,t_0)\frac{d}{dt}\left|\tilde{\Psi}(t)\right\rangle\right] &= [H_0+\lambda W(t)]\,T_0(t,t_0)\left|\tilde{\Psi}(t)\right\rangle, \\ i\hbar\,T_0(t,t_0)\frac{d}{dt}\left|\tilde{\Psi}(t)\right\rangle &= \lambda W(t)\,T_0(t,t_0)\left|\tilde{\Psi}(t)\right\rangle, \\ i\hbar\frac{d}{dt}\left|\tilde{\Psi}(t)\right\rangle &= T_0^{-1}(t,t_0)\lambda W(t)\,T_0(t,t_0)\left|\tilde{\Psi}(t)\right\rangle \\ &\equiv \lambda\tilde{W}(t)\left|\tilde{\Psi}(t)\right\rangle. \end{aligned}$$

This can now be formally integrated to yield

$$\begin{aligned} \left|\tilde{\Psi}(t)\right\rangle &= \exp\left(\frac{-i}{\hbar}\int_{t_0}^{t} dt'\,\lambda\tilde{W}(t')\right)\left|\tilde{\Psi}(t_0)\right\rangle \\ &\equiv \tilde{T}(t,t_0)\left|\tilde{\Psi}(t_0)\right\rangle, \end{aligned}$$

where $\tilde{T}(t,t_0)$ is the unitary time-development operator in the Interaction Picture. This can, in general, be still too difficult to solve!

For infinitesimal time increments however,

$$
\begin{aligned}
i\hbar \frac{d}{dt} \left| \tilde{\Psi}(t) \right\rangle &= \lambda \tilde{W}(t) \left| \tilde{\Psi}(t) \right\rangle, \\
\left| \tilde{\Psi}(t+dt) \right\rangle - \left| \tilde{\Psi}(t) \right\rangle &= \frac{-i}{\hbar} \lambda \tilde{W}(t) \left| \tilde{\Psi}(t) \right\rangle dt, \\
\left| \tilde{\Psi}(t+dt) \right\rangle &= \left[1 - \frac{i}{\hbar} \lambda \tilde{W}(t)\, dt \right] \left| \tilde{\Psi}(t) \right\rangle, \\
\tilde{T}(t+dt,t) &= 1 - \frac{i}{\hbar} \lambda \tilde{W}(t)\, dt \\
&= \tilde{T}(t,t) - \frac{i}{\hbar} \lambda \tilde{W}(t)\, dt, \\
\tilde{T}(t+dt,t) - \tilde{T}(t,t) &= -\frac{i}{\hbar} \lambda \tilde{W}(t)\, dt.
\end{aligned}
$$

On the LHS of the last line we recognize

$$
\tilde{T}(t+dt,t) - \tilde{T}(t,t) \equiv d\left[\tilde{T}(t,t) \right].
$$

Using the semigroup property

$$
\tilde{T}(t+dt,t_0) = \tilde{T}(t+dt,t)\tilde{T}(t,t_0),
$$

we have

$$
\begin{aligned}
d\left[\tilde{T}(t,t_0) \right] &= \tilde{T}(t+dt,t_0) - \tilde{T}(t,t_0) \\
&= \tilde{T}(t+dt,t)\tilde{T}(t,t_0) - \tilde{T}(t,t)\tilde{T}(t,t_0) \\
&= d\left[\tilde{T}(t,t) \right] \tilde{T}(t,t_0) \\
&= -\frac{i}{\hbar} \lambda \tilde{W}(t) \tilde{T}(t,t_0)\, dt
\end{aligned}
$$

as the differential equation for $\tilde{T}(t,t_0)$. Integrating, we find

$$
\begin{aligned}
\int_{t_0}^{t} d\left[\tilde{T}(t',t_0) \right] &= -\frac{i}{\hbar} \int_{t_0}^{t} \lambda \tilde{W}(t') \tilde{T}(t',t_0)\, dt', \\
\tilde{T}(t,t_0) - 1 &= -\frac{i}{\hbar} \int_{t_0}^{t} \lambda \tilde{W}(t') \tilde{T}(t',t_0)\, dt', \\
\tilde{T}(t,t_0) &= 1 - \lambda \frac{i}{\hbar} \int_{t_0}^{t} \tilde{W}(t') \tilde{T}(t',t_0)\, dt'.
\end{aligned}
$$

To derive a perturbation expansion, we suppose that $\tilde{T}(t,t_0)$ takes the form

$$
\begin{aligned}
\tilde{T}(t,t_0) &= \exp\left(\frac{-i}{\hbar} \int_{t_0}^{t} dt' \, \lambda \tilde{W}(t') \right) \\
&= \sum_{n=0}^{\infty} \lambda^n \tilde{T}_n(t,t_0).
\end{aligned}
$$

Plugging this expansion into the above integral equation, we find

$$
\begin{aligned}
\tilde{T}(t,t_0) &= 1 - \lambda \frac{i}{\hbar} \int_{t_0}^{t} \tilde{W}(t') \tilde{T}(t',t_0)\, dt', \\
\sum_{n=0}^{\infty} \lambda^n \tilde{T}_n(t,t_0) &= 1 - \lambda \frac{i}{\hbar} \int_{t_0}^{t} \tilde{W}(t') \left[\sum_{n=0}^{\infty} \lambda^n \tilde{T}_n(t',t_0) \right] dt'.
\end{aligned}
$$

Equating powers of λ, we obtain the recursion

$$
\begin{aligned}
\tilde{T}_0(t,t_0) &= 1, \\
\tilde{T}_{n+1}(t,t_0) &= -\frac{i}{\hbar} \int_{t_0}^{t} \tilde{W}(t') \tilde{T}_n(t',t_0)\, dt'.
\end{aligned}
$$

Hence

$$
\begin{aligned}
\tilde{T}_0(t,t_0) &= 1, \\
\tilde{T}_0(t,t_0) + \lambda\tilde{T}_1(t,t_0) &= 1 - \lambda\frac{i}{\hbar}\int_{t_0}^{t}\tilde{W}(t')\,dt', \\
\tilde{T}_0(t,t_0) + \lambda\tilde{T}_1(t,t_0) + \lambda^2\tilde{T}_2(t,t_0) &= 1 - \lambda\frac{i}{\hbar}\int_{t_0}^{t}\tilde{W}(t')\,dt' - \lambda^2\frac{i}{\hbar}\int_{t_0}^{t}\tilde{W}(t')\left[-\frac{i}{\hbar}\int_{t_0}^{t'}\tilde{W}(t'')\,dt''\right]dt' \\
&= 1 - \lambda\frac{i}{\hbar}\int_{t_0}^{t}\tilde{W}(t')\,dt' + \left(\frac{-i}{\hbar}\right)^2\int_{t_0}^{t}\lambda\tilde{W}(t')\,dt'\int_{t_0}^{t'}\lambda\tilde{W}(t'')\,dt'' \\
\vdots &= \vdots,
\end{aligned}
$$

which we may recognize as an iterative scheme for solution of the integral equation for $\tilde{T}(t,t_0)$.

First-order transition probabilities

Using the result above, we obtain the first-order approximation

$$
\begin{aligned}
\langle k|T(t,t_0)|s\rangle = \left\langle \tilde{k}|\tilde{T}(t,t_0)|\tilde{s}\right\rangle &\approx \delta_{ks} - \frac{i}{\hbar}\int_{t_0}^{t}\left\langle \tilde{k}|\lambda\tilde{W}(t')|\tilde{s}\right\rangle dt' \\
&= \delta_{ks} - \frac{i}{\hbar}\int_{t_0}^{t}\langle k|T_0(t,t_0)T_0^{-1}(t',t_0)\lambda W(t')\,T_0(t',t_0)T_0^{-1}(t,t_0)|s\rangle\,dt' \\
&= \delta_{ks} - \frac{i}{\hbar}\exp[-i\omega_{ks}(t-t_0)]\int_{t_0}^{t}\langle k|T_0^{-1}(t',t_0)\lambda W(t')\,T_0(t',t_0)|s\rangle\,dt' \\
&= \delta_{ks} - \frac{i}{\hbar}\exp[-i\omega_{ks}(t-t_0)]\int_{t_0}^{t}\langle k|\lambda W(t')|s\rangle\exp(i(E_k-E_s)(t'-t_0)/\hbar)dt' \\
&= \delta_{ks} - \frac{i}{\hbar}\exp[-i\omega_{ks}(t-t_0)]\int_{t_0}^{t}\langle k|\lambda W(t')|s\rangle\exp(i\omega_{ks}(t'-t_0))dt' \\
&= \delta_{ks} - \frac{i}{\hbar}\exp(-i\omega_{ks}t)\int_{t_0}^{t}\langle k|\lambda W(t')|s\rangle\exp(i\omega_{ks}t')dt'
\end{aligned}
$$

and consequently, for $k \neq s$ the transition probabilities are

$$
\begin{aligned}
P_{k\leftarrow s}(t) &= |\langle k|T(t,t_0)|s\rangle|^2 \\
&\approx \frac{1}{\hbar^2}\left|\int_{t_0}^{t}\langle k|\lambda W(t')|s\rangle\exp(i\omega_{ks}t')dt'\right|^2.
\end{aligned}
$$

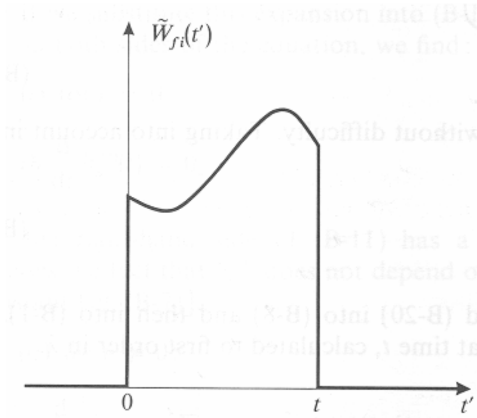
In the common case where $W(t)$ is non-zero only within a finite interval $[t_f, t_i]$ we may speak of “total” transition probabilities for $t \gg t_f$, which may be expressed with limits of integration that are taken to $\pm\infty$:

$$
P_{k\leftarrow s}(\infty) \approx \frac{1}{\hbar^2}\left|\int_{-\infty}^{+\infty}\langle k|\lambda W(t')|s\rangle\exp(i\omega_{ks}t')dt'\right|^2.
$$

Here we recognize the mod-square of the Fourier component of the perturbation matrix element at the relevant Bohr frequency. Similarly, for a general situation where the perturbation suddenly turns on at t_0 and we are interested in the transition probabilities at time t, $P_{k\leftarrow s}(t)$ is given by the Fourier transform of a windowed version of $\langle k|\lambda W(t)|s\rangle$:

$$
\begin{aligned}
P_{k\leftarrow s}(t) &\approx \frac{1}{\hbar^2}\left|\int_{t_0}^{t}\langle k|\lambda W(t')|s\rangle \exp(i\omega_{ks}t')dt'\right|^2 \\
&= \frac{1}{\hbar^2}\left|\int_{-\infty}^{+\infty}\langle k|\lambda W'(t')|s\rangle \exp(i\omega_{ks}t')dt'\right|^2, \\
W'(t) &= W(t)\theta(t,t_0),
\end{aligned}
$$

where $\theta(t,t_0)$ is a function equal to one in the time interval $t_0 \to t$ and zero otherwise [C-T *et al*, Ch. XIII Fig. 1]:



Hence even if $W(t)$ is trying to be a narrow-band perturbation (that is, having a very narrow Fourier transform) we see that at short times t its effective spectral distribution must generally be as broad as $\sim (t - t_0)^{-1}$.

Sinusoidal or constant perturbations

Suppose the perturbation $W(t)$ takes the form

$$
\begin{aligned}
W(t) &= W_0 \cos\omega t \\
&= \frac{W_0}{2}(\exp(+i\omega t) + \exp(-i\omega t)).
\end{aligned}
$$

which includes constant perturbations in the limit $\omega \to 0$. Then our first-order transition probabilities will have the form (setting now $t_0 \equiv 0$)

$$
\begin{aligned}
P_{k\leftarrow s}(t) &\approx \frac{1}{\hbar^2}\left|\int_0^t\langle k|\lambda W(t')|s\rangle \exp(i\omega_{ks}t')dt'\right|^2 \\
&= \frac{\lambda^2}{4\hbar^2}\left|\int_0^t\langle k|W_0|s\rangle(\exp(+i\omega t') + \exp(-i\omega t'))\exp(i\omega_{ks}t')dt'\right|^2 \\
&= \frac{\lambda^2}{4\hbar^2}|\langle k|W_0|s\rangle|^2\left|\int_0^t \exp(i(\omega_{ks}+\omega)t')\,dt' + \int_0^t \exp(i(\omega_{ks}-\omega)t')dt'\right|^2 \\
&= \frac{\lambda^2}{4\hbar^2}|\langle k|W_0|s\rangle|^2\left|\frac{\exp[i(\omega_{ks}+\omega)t]-1}{i(\omega_{ks}+\omega)} + \frac{\exp[i(\omega_{ks}-\omega)t]-1}{i(\omega_{ks}-\omega)}\right|^2 \\
&= \frac{\lambda^2|\langle k|W_0|s\rangle|^2}{4\hbar^2}\left|\frac{\exp[i(\omega_{ks}+\omega)t]-1}{(\omega_{ks}+\omega)} + \frac{\exp[i(\omega_{ks}-\omega)t]-1}{(\omega_{ks}-\omega)}\right|^2.
\end{aligned}
$$

If we focus for the moment on the $\omega = 0$ case, we have

$$\begin{aligned} P_{k\leftarrow s}(t) &\approx \frac{\lambda^2|\langle k|W_0|s\rangle|^2}{4\hbar^2}\left|\frac{\exp[i\omega_{ks}t]-1}{\omega_{ks}}+\frac{\exp[i\omega_{ks}t]-1}{\omega_{ks}}\right|^2 \\ &= \frac{\lambda^2|\langle k|W_0|s\rangle|^2}{\hbar^2}\left|\frac{\exp[i\omega_{ks}t]-1}{\omega_{ks}}\right|^2 \\ &= \frac{\lambda^2|\langle k|W_0|s\rangle|^2}{\hbar^2}\left(\frac{\exp[i\omega_{ks}t]-1}{\omega_{ks}}\right)\left(\frac{\exp[-i\omega_{ks}t]-1}{\omega_{ks}}\right) \\ &= \frac{\lambda^2|\langle k|W_0|s\rangle|^2}{\hbar^2}\left[\frac{1-\exp[i\omega_{ks}t]-\exp[-i\omega_{ks}t]+1}{\omega_{ks}^2}\right] \\ &= \frac{\lambda^2|\langle k|W_0|s\rangle|^2}{\hbar^2}\left[\frac{2-2\cos(\omega_{ks}t)}{\omega_{ks}^2}\right]. \end{aligned}$$

Using the half-angle formula

$$1-\cos\alpha = 2\sin^2\frac{\alpha}{2},$$

we have

$$\begin{aligned} P_{k\leftarrow s}(t) &\approx \frac{\lambda^2|\langle k|W_0|s\rangle|^2}{\hbar^2}\left[\frac{\sin(\omega_{ks}t/2)}{\omega_{ks}/2}\right]^2 \\ &\equiv \frac{\lambda^2|\langle k|W_0|s\rangle|^2}{\hbar^2}\mathsf{F}(t,\omega_{ks}), \end{aligned}$$

which will serve as a definition for $\mathsf{F}(t,\omega_{ks})$.

Getting back to the case of finite ω, we can obtain a very similar form for $P_{k\leftarrow s}(t)$ near resonance. We have seen from the Fourier-transform argument that this transition probability should only be appreciable when $\omega \sim \omega_{ks}$. In that case our first-order expression

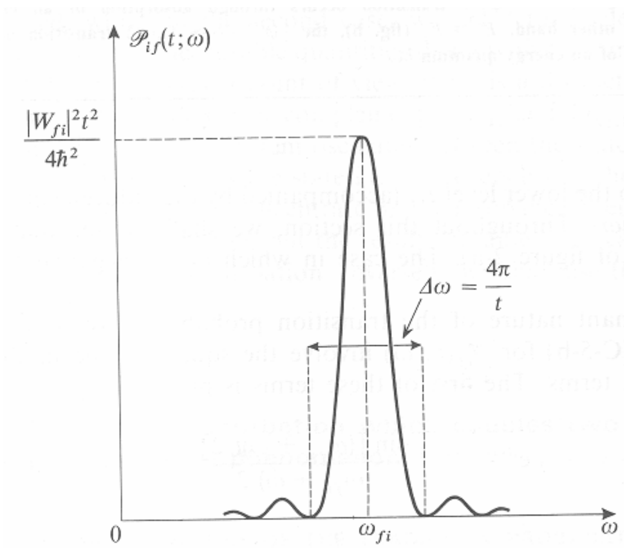
$$P_{k\leftarrow s}(t) \approx \frac{\lambda^2|\langle k|W_0|s\rangle|^2}{4\hbar^2}\left|\frac{\exp[i(\omega_{ks}+\omega)t]-1}{(\omega_{ks}+\omega)}+\frac{\exp[i(\omega_{ks}-\omega)t]-1}{(\omega_{ks}-\omega)}\right|^2$$

contains one clearly dominant term, with $\omega_{ks}-\omega \sim 0$ in the denominator. Then

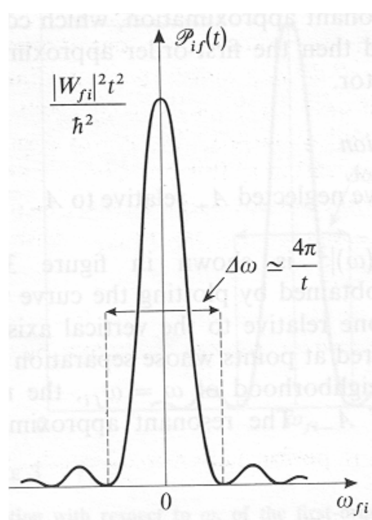
$$\begin{aligned} P_{k\leftarrow s}(t) &\approx \frac{\lambda^2|\langle k|W_0|s\rangle|^2}{4\hbar^2}\left|\frac{\exp[i(\omega_{ks}-\omega)t]-1}{(\omega_{ks}-\omega)}\right|^2 \\ &= \frac{\lambda^2|\langle k|W_0|s\rangle|^2}{4\hbar^2}\mathsf{F}(t,\omega-\omega_{ks}), \end{aligned}$$

by following the same steps as above.

Let us now consider what the transition probability will be at a fixed time t, but for a range of values of ω (around resonance) [C-T *et al*, Ch. XIII Fig. 3]:



For constant perturbations we have a similar picture [C-T *et al*, Ch. XIII Fig. 4]:



Note that the width of the large central peak of this modified sync-function (in either case) becomes more and more narrow with increasing t, while the height of it increases as t^2 (which can be derived, for example, by Taylor expanding F$(t,\omega - \omega_{ks})$ and taking the limit $\omega \to \omega_{ks}$).

When thinking about these expressions it is important to remember that our first-order perturbative treatment is only valid so long as $P_{k\leftarrow s}(t) \ll 1$. In addition the resonant approximation used for the sinusoidal case requires that we be able to neglect the $(\omega + \omega_{ks})^{-1}$ term in favor of the $(\omega - \omega_{ks})^{-1}$, which if you think about it in terms of sync-functions localized at $\pm\omega_{ks}$ leads to the further condition

$$t \gg \frac{1}{\omega_{ks}} \sim \frac{1}{\omega}.$$

Hence, it seems that our picture has a limited time-window of validity, for times not too short (resonance approximation) and not too long (small transition probabilities).