Summary of time dependent theory equations

Time dependent perturbation expansion

Now suppose that the perturbation depends on time, \( \mathcal{H}(r,t) = \mathcal{H}_0(r) + \mathcal{H}_1(r,t) \). The differential equation we must solve is

\[
i\hbar \frac{\partial \Phi(r,t)}{\partial t} = \mathcal{H}(r,t) \Phi(r,t).
\] (1)

We will again assume that we know all of the eigenvalues and eigenfunctions of the reference Hamiltonian

\[
\mathcal{H}_0 \Phi_n^0 = E_n^0 \Phi_n^0.
\] (2)

In this case, the time dependence of the zero order eigenfunctions takes the form:

\[
\Phi_n^0(r,t) = \phi_n^0(r)e^{-iE_n^0 t/\hbar}.
\] (3)

The spatial functions \( \phi_n^0(r) \) form a complete orthonormal set of functions. The full solution is expected to take the form

\[
\Phi(r,t) = \sum_n a_n(t) \phi_n^0(r)e^{-iE_n^0 t/\hbar},
\] (4)

where the coefficients \( a_n(t) \) are to be determined from solution of the first order differential equation:

\[
\frac{d a_n(t)}{dt} = \frac{1}{i\hbar} \sum_m a_m(t) e^{i(E_n^0 - E_m^0) t/\hbar} \langle \phi_m^0 | \mathcal{H}_1 | \phi_n^0 \rangle.
\] (5)

At this point, we have not made any approximations. In order to proceed, we expand the coefficients as a sum of orders of approximation:

\[
a_n(t) = a_n^{(0)}(t) + a_n^{(1)}(t) + a_n^{(2)}(t) + \ldots.
\] (6)

In general we will assume that the system is initially in a well-defined state of the zero order Hamiltonian:

\[
a_m^{(0)}(t) = \delta_{nm}.
\] (7)

The equation for the first order coefficient then takes the form:

\[
a_n^{(1)}(t) = \frac{1}{i\hbar} \int_{-\infty}^{t} dt' e^{i(E_n^0 - E_m^0) t'/\hbar} \langle \phi_n^0 | \mathcal{H}_1 | \phi_m^0 \rangle(t').
\] (8)

Thus the first order coefficients can be determined from a knowledge of the matrix elements of the time-dependent perturbation \( \mathcal{H}_1(r,t) \). Higher order corrections can be determined from the lower order coefficients.
We will consider the first order coefficients for the case in which there is a harmonic time
dependence which is “turned on” at time $t = 0$:

$$\mathcal{H}_1(r, t) = V(r) \left( e^{i\omega t} + e^{-i\omega t} \right) \Theta(t),$$  \hfill (9)

where $\Theta(t)$ denotes the Heaviside step function. If the system is initially $(t < 0)$ in the zero
order state $\Phi^0_n$, the effects of the perturbation to first order in $V$ is given by

$$\Phi_n(r, t) \approx \phi^0_n(r)e^{-iE^0_n t/\hbar} + \sum_m a^{(1)}_m(t)\phi^0_m(r)e^{-iE^0_m t/\hbar},$$  \hfill (10)

where

$$a^{(1)}_m(t) = -\frac{V_{mn}}{i\hbar} \left[ \frac{e^{i(\omega_{mn} + \omega)t} - 1}{\omega_{mn} + \omega} - \frac{e^{i(\omega_{mn} - \omega)t} - 1}{\omega_{mn} - \omega} \right].$$  \hfill (11)

In this expression, $\omega_{mn} \equiv \frac{E^0_m - E^0_n}{\hbar}$. For large times $t$, it can be shown that the squared
modulus of the excitation coefficient $a^{(1)}_m(t)$ determines the transition rate:

$$R_{n \rightarrow m} = \frac{|a^{(1)}_m(t)|^2}{t} \approx \frac{2\pi}{\hbar^2} |V_{mn}|^2 (\delta(\omega_{mn} + \omega) + \delta(\omega_{mn} - \omega)),$$  \hfill (12)

or

$$R_{n \rightarrow m} \approx \frac{2\pi}{\hbar} |V_{mn}|^2 \left( \delta(E^0_m - E^0_n + \hbar \omega) + \delta(E^0_m - E^0_n - \hbar \omega) \right).$$  \hfill (13)