Summary of perturbation theory equations

Time independent perturbation expansion

Suppose we have a reference Hamiltonian $\mathcal{H}_0$ for which we know all of the eigenvalues and eigenfunctions:

$$\mathcal{H}_0 \phi_n^0 = E_n^0 \phi_n^0. \quad (1)$$

Now we want to approximate the eigenvalues $E_n$ and eigenfunctions $\Phi_n$ of total Hamiltonian $\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1$, where the second term is small compared to the reference Hamiltonian term. If the $n^{th}$ zero-order eigenstate ($E_n^0$) is not degenerate, then we can make the following expansion. We will use the shorthand notation $\langle \Phi_n^k | \mathcal{H}_1 | \Phi_m^0 \rangle \equiv V_{km}$.

$$E_n \approx E_n^0 + V_{nn} + \sum_{m \neq n} \frac{|V_{mn}|^2}{E_n^0 - E_m^0} + O(V^3). \quad (2)$$

$$\Phi_n \approx \phi_n^0 + \sum_{m \neq n} \Phi_m^0 \frac{V_{mn}}{E_n^0 - E_m^0} + O(V^2). \quad (3)$$

If, on the other hand, the zero-order eigenstate ($E_n^0$) is degenerate with one or more other eigenstates, another method must be used. Suppose there are $N$ such degenerate states which we will label $\{\phi_n^{i0}\}$, where $i = 1, 2, \ldots, N$. We suppose that we can find $N$ new zero-order states $\{\Phi_i^{\alpha}\}$ from linear combinations of the original states, by diagonalizing the following $N \times N$ matrix:

$$\begin{pmatrix} E_{n_1}^0 + V_{n_1n_1} & V_{n_1n_2} & V_{n_1n_3} & \cdots & V_{n_1n_N} \\ V_{n_2n_1} & E_{n_2}^0 + V_{n_2n_2} & V_{n_2n_3} & \cdots & V_{n_2n_N} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ V_{n_Nn_1} & V_{n_Nn_2} & V_{n_Nn_3} & \cdots & E_{n_N}^0 + V_{n_Nn_N} \end{pmatrix} \begin{pmatrix} C_{n_1}^\alpha \\ C_{n_2}^\alpha \\ \vdots \\ C_{n_N}^\alpha \end{pmatrix} = E^\alpha \begin{pmatrix} C_{n_1}^\alpha \\ C_{n_2}^\alpha \\ \vdots \\ C_{n_N}^\alpha \end{pmatrix} \quad (4)$$

The energy eigenvalues $\{E^\alpha\}$ correspond to corrections up to first order in the perturbation for this system. Each eigenvalue $E^\alpha$ corresponds to a linear combination of the zero order eigenfunctions in terms of the coefficients $\{C_{n_i}^\alpha\}$:

$$\phi_n^{0\alpha} = \sum_{i=1}^N C_{n_i}^\alpha \phi_n^{i0}. \quad (5)$$
Time dependent perturbation expansion

Now suppose that the perturbation depends on time. We will focus on the case in which there is a harmonic time dependence which is “turned on” at time \( t = 0 \):

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

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

\[
\Phi_n(r, t) \approx \Phi_n^0(r) e^{-iE_n^0 t/\hbar} + \sum_m c_m^{(1)}(t) \Phi_m^0(r) e^{-iE_m^0 t/\hbar},
\]

where

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

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

\[
R_{n \rightarrow m} = \frac{|c_m^{(1)}(t)|^2}{t} \approx \frac{2\pi}{\hbar^2} |V_{mn}|^2 \left( \delta(\omega_{mn} + \omega) + \delta(\omega_{mn} - \omega) \right),
\]

or

\[
R_{n \rightarrow m} \approx \frac{2\pi}{\hbar} |V_{mn}|^2 \left( \delta(E_m^0 - E_n^0 + \hbar \omega) + \delta(E_m^0 - E_n^0 - \hbar \omega) \right),
\]