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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:

$$\mathcal{H}_0 \Phi_n^0 = E_n^0 \Phi_n^0. \tag{1}$$

Now we want to approximate the eigenvalues E_n and eigenfunctions Φ_n of total Hamiltonian $\mathcal{H} \equiv \mathcal{H}_0 + \mathcal{H}_1$, 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 $\langle \Phi_k^0 | \mathcal{H}_1 | \Phi_m^0 \rangle \equiv V_{km}$.

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

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

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 $\{\Phi_{n_i}^0\}$, where $i = 1, 2, \ldots N$. We suppose that we can find N new zero-order states $\{\Phi^{0\alpha}\}$ from linear combinations of the original states, by diagonalizing the following $N \times N$ matrix:

$$\begin{pmatrix} E_{n_1}^0 + V_{n_1 n_1} & V_{n_1 n_2} & V_{n_1 n_3} & \ldots & V_{n_1 n_N} \\ V_{n_2 n_1} & E_{n_2}^0 + V_{n_2 n_2} & V_{n_2 n_3} & \ldots & V_{n_3 n_N} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ V_{n_N n_1} & V_{n_N n_3} & V_{n_N n_3} & \ldots & E_{n_N}^0 + V_{n_N n_N} \end{pmatrix} \begin{pmatrix} C_{n_1}^\alpha \\ C_{n_2}^\alpha \\ \vdots \\ C_{n_N}^\alpha \end{pmatrix} = E^\alpha \begin{pmatrix} C_{n_1}^\alpha \\ C_{n_2}^\alpha \\ \vdots \\ C_{n_N}^\alpha \end{pmatrix} \tag{4}$$

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

$$\Phi^{0\alpha} = \sum_{i=1}^{N} C_{n_i}^\alpha \Phi_{n_i}^0. \tag{5}$$

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 $t = 0$:

$$\mathcal{H}_1(t) = V(\mathbf{r}) \left(\mathrm{e}^{i\omega t} + \mathrm{e}^{-i\omega t} \right) \Theta(t), \tag{6}$$

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

$$\Phi_n(\mathbf{r}, t) \approx \Phi_n^0(\mathbf{r}) \mathrm{e}^{-iE_n^0 t/\hbar} + \sum_m c_m^{(1)}(t) \Phi_m^0(\mathbf{r}) \mathrm{e}^{-iE_m^0 t/\hbar}, \tag{7}$$

where

$$c_m^{(1)}(t) = -\frac{V_{mn}}{\hbar} \left[\frac{\mathrm{e}^{i(\omega_{mn}+\omega)t} - 1}{\omega_{mn} + \omega} + \frac{\mathrm{e}^{i(\omega_{mn}-\omega)t} - 1}{\omega_{mn} - \omega} \right]. \tag{8}$$

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 exitation coefficient $c_m^{(1)}(t)$ determines the transition rate:

$$R_{n \to m} = \frac{|c^(1)_m(t)|^2}{t} \approx \frac{2\pi}{\hbar^2} |V_{mn}|^2 \left(\delta(\omega_{mn} + \omega) + \delta(\omega_{mn} - \omega) \right), \tag{9}$$

or

$$R_{n \to m} \approx \frac{2\pi}{\hbar} |V_{mn}|^2 \left(\delta(E_m^0 - E_n^0 + \hbar\omega) + \delta(E_m^0 - E_n^0 - \hbar\omega) \right), \tag{10}$$