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Summary of time dependent theory equations

Time dependent perturbation expansion

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

$$i\hbar \frac{\partial \Phi(\mathbf{r},t)}{\partial t} = \mathcal{H}(\mathbf{r},t)\Phi(\mathbf{r},t). \tag{1}$$

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

$$\mathcal{H}_0 \Phi_n^0 = E_n^0 \Phi_n^0. \tag{2}$$

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

$$\Phi_n^0(\mathbf{r},t) = \phi_n^0(\mathbf{r}) \mathrm{e}^{-iE_n^0 t/\hbar}. \tag{3}$$

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

$$\Phi(\mathbf{r},t) = \sum_n a_n(t) \phi_n^0(\mathbf{r}) \mathrm{e}^{-iE_n^0 t/\hbar}, \tag{4}$$

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

$$\frac{da_n(t)}{dt} = \frac{1}{i\hbar} \sum_m a_m(t) \mathrm{e}^{i(E_n^0 - E_m^0)t/\hbar} \langle \phi_n^0 | \mathcal{H}_1 | \phi_m^0 \rangle. \tag{5}$$

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

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

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

$$a_m^{(0)}(t) = \delta_{nm}. \tag{7}$$

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

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

Thus the first order coefficients can be determined from a knowledge of the matrix elements of the time-dependent perturbation $\mathcal{H}_1(\mathbf{r},t)$. 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 $t = 0$:

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

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

$$\Phi_n(\mathbf{r}, t) \approx \phi_n^0(\mathbf{r})\mathrm{e}^{-iE_n^0 t/\hbar} + \sum_m a_m^{(1)}(t)\phi_m^0(\mathbf{r})\mathrm{e}^{-iE_m^0 t/\hbar}, \tag{10}$$

where

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

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 $a_m^{(1)}(t)$ determines the transition rate:

$$R_{n\to m} = \frac{|a_m^{(1)}(t)|^2}{t} \approx \frac{2\pi}{\hbar^2}|V_{mn}|^2 \left(\delta(\omega_{mn} + \omega) + \delta(\omega_{mn} - \omega) \right), \tag{12}$$

or

$$R_{n\to m} \approx \frac{2\pi}{\hbar}|V_{mn}|^2 \left(\delta(E_m^0 - E_n^0 + \hbar\omega) + \delta(E_m^0 - E_n^0 - \hbar\omega) \right). \tag{13}$$