Perturbation Theory 2

1 Time-dependent Perturbation

1.1 Generalization

When the perturbation Hamiltonian H' is dependent of time t, we need to deal with the problem in a way that is completely different from that of time-independent case. In this case, we deal with the time dependent Schrodinger's equation.

$$i\hbar\frac{\partial\psi}{\partial t} = (H_0 + H'(t))\psi \tag{1}$$

Assume the solution to be:

$$\psi_n(t) = \sum_m \phi_m e^{-iw_m^{(0)}t} U_{mn}(t) \tag{2}$$

ϕ_m is the eigenstate of the unperturbed Hamiltonian, and $\phi_m e^{-iw_m^{(0)}t}$ is the time dependent eigenstate when $H'(t) \equiv 0$.

$$H_0\phi_m = \hbar w_m^{(0)}\phi_m \tag{3}$$

Substitute (2) into (1) to organize the equation:

$$\frac{d}{dt}U_{mn}(t) = \frac{1}{i\hbar}\sum_k H'_{mk}(t)U_{kn}(t) \tag{4}$$

$$H'_{mk}(t) = \int \phi_m^* e^{iw_m^{(0)}t} H'(t)\phi_k e^{-iw_k^0 t} d^3r \tag{5}$$

In principal, (5) is calculated, hence (4) can be solved by $H'_{mk}(t)$ a known function.

1.2 Sequential Approximation

The equation (4) is consecutively solved under the initial condition (6):

$$t = -\infty \qquad U_{mn}(-\infty) = \delta_{m,n} \tag{6}$$

Ignore $H'_{mk}(t)$ on the right side, then:

$$U_{mn}^{(0)}(t) = \delta_{m,n} \tag{7}$$

Substitute this $U^{(0)}$ for the right side of the equation to integrate:

$$U_{mn}^{(1)}(t) = \delta_{m,n} - \frac{i}{\hbar}\int_{-\infty}^{t} H'_{mn}(t')dt' \tag{8}$$

Further, substitute $U^{(1)}$ into the right side equation of (4) to obtain the following equation:

$$U_{mn}^{(2)}(t) = \delta_{m,n} - \frac{i}{\hbar}\int_{-\infty}^{t} H'_{mn}(t')dt' + (\frac{-i}{\hbar})^2 \sum_k \int_{-\infty}^{t} H'_{mk}(t')dt' \int_{-\infty}^{t'} H'_{kn}(t'')dt'' \tag{9}$$

Limiting Cases:

Constant perturbations

We consider the perturbed Hamiltonian, which is constant, but switched-on at $t=0$:

$$H' = \begin{cases} 0 & : t < 0 \\ H'(\text{一定}) & : t > 0 \end{cases} \tag{10}$$

From the equation (8), we obtain:

$$U^{(1)}_{mn}(t) = \delta_{m,n} + \frac{H'_{mn}}{\hbar}\frac{1 - e^{iw^{(0)}_{mn}(t)}}{w^{(0)}_{mn}} \tag{11}$$

where $H'_{mn} = \langle\phi_m|H'|\phi_n\rangle$. Then we can obtain

$$|U^{(1)}_{mn}(t)|^2 = |H'_{mn}|^2\frac{4\sin^2 w^{(0)}_{mn}t/2}{(\hbar w^{(0)}_{mn})^2} \tag{12}$$

Now, using the equation followings will yield:

$$\lim_{t\to\infty}\frac{\sin(xt)}{x} = \pi\delta(x) \tag{13}$$

$$\frac{4\sin^2(wt/2)}{(\hbar w)^2} = \frac{1}{\hbar^2}\frac{4\sin^2(wt/2)}{4(w/2)^2} = \frac{1}{\hbar^2}t\pi\delta(\frac{w}{2}) = t\frac{2\pi}{\hbar^2}\delta(w) \qquad (t\to\infty) \tag{14}$$

There is a consecutive distribution of transitioned states, and we assume the number of states in between $E \sim E+\Delta E$ to be given by $\rho(E)\Delta E$. Here $\rho(E)$ is called the state density. In this case, the transition probability per a unit time is calculated as:

$$\begin{aligned} w_{m\leftarrow n} &= \lim_{t\to\infty}\frac{1}{t}\frac{|H'_{mn}|^2}{\hbar^2}\int_E^{E+\Delta E} dE^{(0)}_m\rho(E^{(0)}_m)\frac{4\sin^2(w^{(0)}_{mn}t/2)}{(w^{(0)}_{mn})^2} \\ &= \frac{2\pi}{\hbar}|H'_{mn}|^2\rho(E^{(0)}_m) \quad , \quad (E^{(0)}_n = E^{(0)}_m) \end{aligned} \tag{15}$$

The above implies the transitions occur only among states possessing the same energy.

Sinusoidal perturbation

Let us now consider the electromagnetic field that oscillates:

$$H' = \begin{cases} 0 & : t < 0 \\ Fe^{iwt} + F^*e^{-iwt} & : t > 0 \end{cases} \tag{16}$$

$U^{(1)}(t)$ can be calculated in the same manner we did in above:

$$U^{(1)}_{mn}(t) = \delta_{mn} + F^*_{nm}\frac{1 - e^{i(w^{(0)}_{mn}-w)t}}{\hbar(w^{(0)}_{mn} - w)} + F_{mn}\frac{1 - e^{i(w^{(0)}_{mn}+w)t}}{\hbar(w^{(0)}_{mn} + w)} \tag{17}$$

Likewise, the transition probability can be derived in the same way (15):

$$w_{m\leftarrow n} = \frac{2\pi}{\hbar}|F_{mn}|^2\rho(E^{(0)}_m) \quad , \quad E^{(0)}_m - E^{(0)}_n = \pm\hbar w \tag{18}$$

This indicates that among states with different energies, a finite energy is absorbed (or emitted) from oscillating external field and transitions occur.

2 Variation Method

$|0\rangle$: accurate ground states

$|\psi\rangle$: approximational ground states (include a variation parameter)

Expand the state $|\psi\rangle$ as following:

$$|\psi\rangle = \sum_k |k\rangle\langle k|\psi\rangle \tag{19}$$

$|k\rangle$ is the eigenstate of H :

$$H|k\rangle = E_k|k\rangle \tag{20}$$

Thus:

$$H|\psi\rangle = \sum_k E_k|k\rangle\langle k|\psi\rangle \tag{21}$$

To assess this:

$$\frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle} = \frac{\sum_k E_k|\langle k|\psi\rangle|^2}{\sum_k |\langle k|\psi\rangle|^2} = E_0 + \frac{\sum_k (E_k - E_0)|\langle k|\psi\rangle|^2}{\sum_k |\langle k|\psi\rangle|^2} \geq E_0 \tag{22}$$

Therefore, the ground state of the energy E_0 is assessed by the variational wavefunction $|\psi\rangle$:

$$E_0 = \frac{\langle 0|H|0\rangle}{\langle 0|0\rangle} \leq \frac{\langle\psi|H|\psi\rangle}{\langle\psi|\psi\rangle}$$