Perturbation Theory

Consider Hamiltonian of the following form

$$\hat{H}(t) = \hat{H}^{(0)} + \hat{H}^{(1)}(t), \tag{1}$$

where $\hat{H}^{(0)}$ is time-independent and is regarded as being solved with a full set of (eigenvalue, eigenstate) pairs

$$\hat{H}^{(0)} \left|\psi_n^{(0)}\right\rangle = \epsilon_n^{(0)} \left|\psi_n^{(0)}\right\rangle, \tag{2}$$

and $||\hat{H}^{(1)}|| \ll \delta\epsilon^{(0)}$ with $\delta\epsilon^{(0)}$ being the energy level spacing of the unperturbed spectrum [1]. To keep track of the order of the corrections due to $\hat{H}^{(1)}$, we rewrite Eq. (1) as

$$\hat{H}(t, \lambda) = \hat{H}^{(0)} + \lambda \hat{H}^{(1)}(t), \tag{3}$$

and later use λ as an expansion parameter.

Our goal is to find, up to the j-th order correction in λ:

- when $\hat{H}^{(1)}$ is *time-independent*, the (eigenvalue, eigenstate) pairs of the full Hamiltonian:

$$\hat{H}(\lambda) \left|\psi_n(\lambda)\right\rangle = \epsilon_n(\lambda) \left|\psi_n(\lambda)\right\rangle \tag{4}$$

  (λ is set to 1 at the end);

- when $\hat{H}^{(1)}(t)$ is *time-dependent*, the transition probability between unperturbed eigenstates $p_{m\leftarrow n}(t) \equiv \left|\left\langle \psi_m^{(0)} \middle| \hat{U}(t,0) \middle| \psi_n^{(0)} \right\rangle\right|^2$.

[1] The case of degenerate spectrum will be treated separately based on the nondegenerate solution.

1 Time-independent case

We start from formal expansions

$$\epsilon_n(\lambda) = \epsilon_n^{(0)} + \lambda\epsilon_n^{(2)} + \lambda^2\epsilon_n^{(2)} + \cdots\,, \tag{5}$$
$$|\psi_n(\lambda)\rangle = \left|\psi_n^{(0)}\right\rangle + \lambda\left|\psi_n^{(1)}\right\rangle + \lambda^2\left|\psi_n^{(2)}\right\rangle + \cdots\,, \tag{6}$$

where the above kets are not necessarily normalized (which does not affect the validity of Eq. (4)). We will fix, however, $\left|\psi_n^{(0)}\right\rangle$ to be always normalized such that $\left\langle\psi_m^{(0)}|\psi_n^{(0)}\right\rangle = \delta_{mn}$, and in addition $\left|\psi_n^{(j>0)}\right\rangle$ to be always orthogonal to $\left|\psi_n^{(0)}\right\rangle$ such that $\left\langle\psi_n^{(0)}|\psi_n^{(j>0)}\right\rangle = 0$. The latter condition can be seen as absorbing all possible $\left|\psi_n^{(0)}\right\rangle$ components in $\left|\psi_n^{(j>0)}\right\rangle$ into the zero-th order $\left|\psi_n^{(0)}\right\rangle$ (and then renormalize it). The normalization of $|\psi_n(\lambda)\rangle$ comes as the final step by taking $|\psi_n(\lambda)\rangle_{\text{normalized}} = |\psi_n(\lambda)\rangle / \sqrt{\langle\psi_n(\lambda)|\psi_n(\lambda)\rangle}$ and keeping the result up to $O(\lambda^j)$. For example,

$$\text{for } j=1\text{:}\quad |\psi_n(\lambda)\rangle_{\text{normalized}} \simeq \left|\psi_n^{(0)}\right\rangle + \lambda\left|\psi_n^{(1)}\right\rangle; \tag{7}$$
$$\text{for } j=2\text{:}\quad |\psi_n(\lambda)\rangle_{\text{normalized}} \simeq \left(1 - \frac{\lambda^2}{2}\left\langle\psi_n^{(1)}|\psi_n^{(1)}\right\rangle\right)\left|\psi_n^{(0)}\right\rangle + \lambda\left|\psi_n^{(1)}\right\rangle + \lambda^2\left|\psi_n^{(2)}\right\rangle. \tag{8}$$

With the given problem, $\{\left|\psi_n^{(0)}\right\rangle\}$ is obviously "the" basis to work with. Let us use the un-hatted $H^{(0,1)}$ for the matrix representation of $\hat{H}^{(0,1)}$ in this basis:

$$H_{mn}^{(0,1)} = \left\langle\psi_m^{(0)}\right|\hat{H}^{(0,1)}\left|\psi_n^{(0)}\right\rangle, \tag{9}$$

and define matrices $E^{(j)}$ and $\Psi^{(j)}$ with their elements given by

$$E_{mn}^{(j)} = \epsilon_n^{(j)}\delta_{mn}, \quad \Psi_{mn}^{(j)} = \left\langle\psi_m^{(0)}|\psi_n^{(j)}\right\rangle. \tag{10}$$

Note that $E^{(j)}$ *is always diagonal whereas* $\Psi^{(j>0)}$ *always has a vanishing diagonal.*

It follows that Eq. (4) becomes

$$\begin{aligned}&(H^{(0)} + \lambda H^{(1)})(\Psi^{(0)} + \lambda\Psi^{(1)} + \lambda^2\Psi^{(2)} + \cdots)\\ &\quad = (\Psi^{(0)} + \lambda\Psi^{(1)} + \lambda^2\Psi_n^{(2)} + \cdots)(E^{(0)} + \lambda E^{(1)} + \lambda^2 E^{(2)} + \cdots),\end{aligned} \tag{11}$$

where, by construction,

$$H^{(0)} = E^{(0)}, \quad \Psi^{(0)} = \mathbb{1}. \tag{12}$$

Eq. (11) *is the core of the time-independent perturbation theory.* Let us break it down order by order:

$$\begin{aligned}
\lambda^0: \quad & H^{(0)}\Psi^{(0)} = \Psi^{(0)}E^{(0)}; & (13)\\
\lambda^1: \quad & H^{(0)}\Psi^{(1)} + H^{(1)}\Psi^{(0)} = \Psi^{(0)}E^{(1)} + \Psi^{(1)}E^{(0)}; & (14)\\
\lambda^2: \quad & H^{(0)}\Psi^{(2)} + H^{(1)}\Psi^{(1)} = \Psi^{(0)}E^{(2)} + \Psi^{(1)}E^{(1)} + \Psi^{(2)}E^{(0)}; & (15)\\
\lambda^j: \quad & H^{(0)}\Psi^{(j)} + H^{(1)}\Psi^{(j-1)} = \sum_{i=0}^{j} \Psi^{(i)}E^{(j-i)}. & (16)
\end{aligned}$$

As a consequence of the chosen basis, Eq. (13) is as trivial as $E^{(0)}\mathbb{1} = \mathbb{1}E^{(0)}$. Higher order equations become useful. Eq. (14) can be decoupled into diagonal and off-diagonal parts (note that $H^{(0)}\Psi^{(j>0)}$ and $\Psi^{(i>0)}E^{(i')}$ always have vanishing diagonals):

$$\mathrm{diag}(H^{(1)}) = E^{(1)} \quad \text{or} \quad \epsilon_n^{(1)} = H_{nn}^{(1)}; \tag{17}$$

$$\mathrm{offdiag}(E^{(0)}\Psi^{(1)} + H^{(1)}) = \mathrm{offdiag}(\Psi^{(1)}E^{(0)}) \quad \text{or} \quad \Psi_{mn}^{(1)}\big|_{m\neq n} = -\frac{H_{mn}^{(1)}}{\epsilon_m^{(0)} - \epsilon_n^{(0)}}. \tag{18}$$

Similarly, Eq. (15) produces

$$\epsilon_n^{(2)} = \sum_{m\neq n} H_{nm}^{(1)}\Psi_{mn}^{(1)}; \tag{19}$$

$$\Psi_{mn}^{(2)}\big|_{m\neq n} = \frac{\Psi_{mn}^{(1)}H_{nn}^{(1)} - \sum_l H_{ml}^{(1)}\Psi_{ln}^{(1)}}{\epsilon_m^{(0)} - \epsilon_n^{(0)}}. \tag{20}$$

Or, generically,

$$\epsilon_n^{(j)} = (H^{(1)}\Psi^{(j-1)})_{nn} = \left\langle \psi_n^{(0)} \right| \hat{H}^{(1)} \left| \psi_n^{(j-1)} \right\rangle; \tag{21}$$

$$\Psi_{mn}^{(j)}\big|_{m\neq n} = \frac{(\sum_{i=1}^{j-1} \Psi^{(i)}E^{(j-i)} - H^{(1)}\Psi^{(j-1)})_{mn}}{\epsilon_m^{(0)} - \epsilon_n^{(0)}}. \tag{22}$$

The normalization of $\Psi = \sum_{i=0}^{j} \lambda^i \Psi^{(i)}$ is important but straightforward.

2 Time-dependent case

In this section, we shall write $\hat{V}(t) \equiv \hat{H}^{(1)}(t)$ and drop λ because the power of V already indicates the order of the correction. In the interaction picture, with the basis chosen to be $\{\left|\psi_n^{(0)}(t)\right\rangle\}$ with $\left|\psi_n^{(0)}(t)\right\rangle = \hat{U}^{(0)}(t)\left|\psi_n^{(0)}\right\rangle = \exp(-\mathrm{i}\hat{H}^{(0)}t)\left|\psi_n^{(0)}\right\rangle = \exp(-\mathrm{i}\epsilon_n^{(0)}t)\left|\psi_n^{(0)}\right\rangle$, a transition probability amplitudes can be identified (up to a phase factor) with a matrix elements of the interaction time-evolution operator

$$U^I(t)_{mn} = \left\langle\psi_m^{(0)}\right|\hat{U}^I(t)\left|\psi_n^{(0)}\right\rangle = \left\langle\psi_m^{(0)}(t)\right|\hat{U}(t)\left|\psi_n^{(0)}\right\rangle, \tag{23}$$

where

$$\frac{d}{dt}U^I(t) = -\mathrm{i}V^I(t)U^I(t), \tag{24}$$

with

$$V^I_{mn}(t) = \left\langle\psi_m^{(0)}(t)\right|\hat{V}(t)\left|\psi_n^{(0)}(t)\right\rangle = V_{mn}(t)e^{\mathrm{i}(\epsilon_m^{(0)}-\epsilon_n^{(0)})t}. \tag{25}$$

Eq. (24) is formally solved by the Dyson series

$$U^I(t) = \mathbb{1} + (-\mathrm{i})\int_0^t dt_1 V^I(t_1) + (-\mathrm{i})^2\int_0^t dt_1 V^I(t_1)\int_0^{t_1} dt_2 V^I(t_2) + \cdots. \tag{26}$$

Eq. (26) *is the core of the time-dependent perturbation theory.*

To see it at work, let's study the example of the two-level (Rabi) model. In this case, $\epsilon_\pm^{(0)} = \pm\Omega/2$, and

$$V(t) = \begin{pmatrix} 0 & \gamma e^{-\mathrm{i}\omega t} \\ \gamma e^{\mathrm{i}\omega t} & 0 \end{pmatrix} \quad\Rightarrow\quad V^I(t) = \begin{pmatrix} 0 & \gamma e^{\mathrm{i}(\Omega-\omega)t} \\ \gamma e^{-\mathrm{i}(\Omega-\omega)t} & 0 \end{pmatrix}. \tag{27}$$

The first order term in Eq. (26) becomes

$$(-\mathrm{i})\int_0^t dt_1 V^I(t_1) = \begin{pmatrix} 0 & -\frac{\gamma}{\Omega-\omega}[e^{\mathrm{i}(\Omega-\omega)t}-1] \\ \frac{\gamma}{\Omega-\omega}[e^{-\mathrm{i}(\Omega-\omega)t}-1] & 0 \end{pmatrix}. \tag{28}$$

The second order term in Eq. (26) becomes

$$\begin{aligned}&(-\mathrm{i})^2\int_0^t dt_1 V^I(t_1)\int_0^{t_1} dt_2 V^I(t_2) \\ &= \begin{pmatrix} -\mathrm{i}\frac{\gamma^2}{\Omega-\omega}t + (\frac{\gamma}{\Omega-\omega})^2[e^{\mathrm{i}(\Omega-\omega)t}-1] & 0 \\ 0 & \mathrm{i}\frac{\gamma^2}{\Omega-\omega}t + (\frac{\gamma}{\Omega-\omega})^2[e^{-\mathrm{i}(\Omega-\omega)t}-1] \end{pmatrix}.\end{aligned} \tag{29}$$

A Exact solution of the two-level model

In a pre-chosen basis, the model Hamiltonian reads

$$H = \begin{pmatrix} \Omega/2 & \gamma e^{-\mathrm{i}\omega t} \\ \gamma e^{\mathrm{i}\omega t} & -\Omega/2 \end{pmatrix} \qquad (\Omega, \gamma, \omega \geq 0). \tag{30}$$

Let us define

$$\Delta \equiv \sqrt{(\Omega/2)^2 + \gamma^2}, \quad \cos\theta \equiv \frac{\Omega/2}{\Delta}, \quad \sin\theta \equiv \frac{\gamma}{\Delta}, \tag{31}$$

such that

$$H = \Delta \begin{pmatrix} \cos\theta & \sin\theta e^{-\mathrm{i}\omega t} \\ \sin\theta e^{\mathrm{i}\omega t} & -\cos\theta \end{pmatrix}. \tag{32}$$

When $\omega = 0$ (i.e. H is time-independent), the eigenvalues and the corresponding eigenstates are

$$\epsilon_\pm = \pm\Delta, \quad \psi_+ = \begin{pmatrix} \cos\frac{\theta}{2} \\ \sin\frac{\theta}{2} \end{pmatrix}, \quad \psi_- = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix}. \tag{33}$$

If $\gamma \ll \Omega$, we can expand, up to $(\gamma/\Omega)^2$,

$$\Delta \simeq (\Omega/2)\left[1 + \frac{1}{2}\left(\frac{\gamma}{\Omega/2}\right)^2\right] \simeq \frac{\Omega}{2} + \frac{\gamma^2}{\Omega}, \tag{34}$$

$$\cos\frac{\theta}{2} = \sqrt{\frac{1}{2}(1+\cos\theta)} = \sqrt{\frac{1}{2}(1 + \left[1 + \left(\frac{\gamma}{\Omega/2}\right)^2\right]^{-1/2})} \simeq 1 - \frac{1}{2}\left(\frac{\gamma}{\Omega}\right)^2, \tag{35}$$

$$\sin\frac{\theta}{2} = \sqrt{\frac{1}{2}(1-\cos\theta)} = \sqrt{\frac{1}{2}(1 - \left[1 + \left(\frac{\gamma}{\Omega/2}\right)^2\right]^{-1/2})} \simeq \frac{\gamma}{\Omega}. \tag{36}$$

These expansions allow us to compare the exact solutions in Eq. (33) with a time-independent perturbation calculation.

When $\omega > 0$ (i.e. H is time-dependent), we aim to solve for the time-evolution operator $U(t) \equiv U(t, 0)$ which satisfies

$$\frac{d}{dt}U(t) = -\mathrm{i}H(t)U(t). \tag{37}$$

We first transform

$$\tilde{H} = \rho_\omega(t) H(t) \rho_\omega(t)^{-1} = \begin{pmatrix} \Omega/2 & \gamma \\ \gamma & -\Omega/2 \end{pmatrix}, \tag{38}$$

$$\tilde{U}(t) = \rho_\omega(t) U(t), \tag{39}$$

where

$$\rho_\omega(t) \equiv \begin{pmatrix} e^{\mathrm{i}\omega t/2} & \\ & e^{-\mathrm{i}\omega t/2} \end{pmatrix}. \tag{40}$$

Then Eq. (37) becomes

$$\frac{d}{dt}\tilde{U}(t) = -\mathrm{i}(\tilde{H} - \frac{\omega}{2}\sigma_z)\tilde{U}(t). \tag{41}$$

Now we have a time-independent "effective" Hamiltonian such that we immediately obtain

$$\tilde{U}(t) = \exp[-\mathrm{i}(\tilde{H} - \frac{\omega}{2}\sigma_z)t] \tag{42}$$

$$= \cos(\Delta_\omega t) - \mathrm{i}\sin(\Delta_\omega t)(\cos\theta_\omega \sigma_z + \sin\theta_\omega \sigma_x), \tag{43}$$

where

$$\Delta_\omega \equiv \sqrt{(\frac{\Omega - \omega}{2})^2 + \gamma^2}, \quad \cos\theta_\omega \equiv \frac{(\Omega - \omega)/2}{\Delta_\omega}, \quad \sin\theta_\omega \equiv \frac{\gamma}{\Delta_\omega}. \tag{44}$$

If the initial state at $t = 0$ is given by $\psi(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$, then

$$\psi(t) = U(t)\psi(0) = \begin{pmatrix} e^{-\mathrm{i}\omega t/2}[\cos(\Delta_\omega t) - \mathrm{i}\sin(\Delta_\omega t)\cos\theta_\omega] \\ -\mathrm{i}e^{\mathrm{i}\omega t/2}\sin(\Delta_\omega t)\sin\theta_\omega \end{pmatrix}. \tag{45}$$

It follows that the transition probability from the first component to the second is given by

$$p(t) = \sin^2(\Delta_\omega t)\sin^2\theta_\omega = \frac{\gamma^2}{(\frac{\Omega-\omega}{2})^2 + \gamma^2}\sin^2(\Delta_\omega t). \tag{46}$$