Time Independent Perturbation Theory (Non-degenerate)

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Time Independent Perturbation Theory

We consider the known Hamiltonian H^0 with a small perturbation H^1

$$H = H^0 + \lambda H^1.$$

For the original (unperturbed) Hamiltonian, we have all eigenstates and eigenvalues

$$H^0|n^0\rangle = E_n^0|n^0\rangle.$$

Expanding $|n^0\rangle$ and E_n^0, we have

$$\begin{aligned}\left(H^0 + \lambda H^1\right)&\left(|n^0\rangle + \lambda|n^1\rangle + \lambda^2|n^2\rangle + \cdots\right) \\ &= \left(E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots\right)\left(|n^0\rangle + \lambda|n^1\rangle + \lambda^2|n^2\rangle + \cdots\right).\end{aligned}$$

Time Independent Perturbation Theory

$$H^0|n^0\rangle + \lambda[H^1|n^0\rangle + H^0|n^1\rangle] + \lambda^2[H^1|n^1\rangle + H^0|n^2\rangle] + \cdots$$
$$= E_n^0|n^0\rangle + \lambda[E_n^1|n^0\rangle + E_n^0|n^1\rangle] + \lambda^2[E_n^1|n^1\rangle + E_n^0|n^2\rangle + E_n^2|n^0\rangle] + \cdots$$

Then, we have

- 0th: $H^0|n^0\rangle = E_n^0|n^0\rangle$.
- 1th: $H^1|n^0\rangle + H^0|n^1\rangle = E_n^1|n^0\rangle + E_n^0|n^1\rangle$.
- 2th: $H^1|n^1\rangle + H^0|n^2\rangle = E_n^1|n^1\rangle + E_n^0|n^2\rangle + E_n^2|n^0\rangle$.

First Order Correction

From the first order equation,

$$H^1|n^0\rangle + H^0|n^1\rangle = E_n^1|n^0\rangle + E_n^0|n^1\rangle, \tag{1}$$

applying $\langle n^0|$, we have

$$\begin{aligned}\langle n^0|H^1|n^0\rangle + \langle n^0|H^0|n^1\rangle &= \langle n^0|E_n^1|n^0\rangle + \langle n^0|E_n^0|n^1\rangle \\ \langle n^0|H^1|n^0\rangle + E_n^0\langle n^0|n^1\rangle &= E_n^1 + \langle n^0|E_n^0|n^1\rangle.\end{aligned}$$

Therefore, the first order correction is

$$E_n^1 = \langle n^0|H^1|n^0\rangle.$$

First Order Correction

From the first order equation,

$$H^1|n^0\rangle + H^0|n^1\rangle = E_n^1|n^0\rangle + E_n^0|n^1\rangle, \tag{2}$$

applying $\langle m^0|$, we have

$$\begin{aligned}\langle m^0|H^1|n^0\rangle + \langle m^0|H^0|n^1\rangle &= \langle m^0|E_n^1|n^0\rangle + \langle m^0|E_n^0|n^1\rangle \\ \langle m^0|H^1|n^0\rangle + E_m^0\langle m^0|n^1\rangle &= E_n^1\delta_{m,n} + E_n^0\langle m^0|n^1\rangle.\end{aligned}$$

Thus,

$$\langle m^0|n^1\rangle = \frac{\langle m^0|H^1|n^0\rangle}{E_n^0 - E_m^0}.$$

Finally, the first order correction to the wave function is

$$\begin{aligned}|n\rangle = |n^0\rangle + |n^1\rangle &= |n^0\rangle + \sum_m |m^0\rangle\langle m^0|n^1\rangle \\ &= |n^0\rangle + \sum_{m\neq n} \frac{\langle m^0|H^1|n^0\rangle}{E_n^0 - E_m^0}|m^0\rangle.\end{aligned}$$

Second Order Correction

From the second order equation,

$$H^1|n^1\rangle + H^0|n^2\rangle = E_n^1|n^1\rangle + E_n^0|n^2\rangle + E_n^2|n^0\rangle$$

applying $\langle n^0|$, we have

$$\langle n^0|H^1|n^1\rangle + \langle n^0|H^0|n^2\rangle = \langle n^0|E_n^1|n^1\rangle + \langle n^0|E_n^0|n^2\rangle + \langle n^0|E_n^2|n^0\rangle$$
$$\langle n^0|H^1|n^1\rangle + E_n^0\langle n^0|n^2\rangle = \langle n^0|E_n^1|n^1\rangle + E_n^0\langle n^0|n^2\rangle + \langle n^0|E_n^2|n^0\rangle$$
$$\langle n^0|H^1|n^1\rangle = \langle n^0|E_n^1|n^1\rangle + \langle n^0|E_n^2|n^0\rangle$$

Second Order Correction

Thus,

$$
\begin{aligned}
E_n^2 &= \langle n^0 | H^1 | n^1 \rangle - \langle n^0 | E_n^1 | n^1 \rangle \\
&= \langle n^0 | H^1 | n^1 \rangle - E_n^1 \langle n^0 | n^1 \rangle \\
&= \langle n^0 | H^1 | n^1 \rangle - E_n^1 \sum_{m \neq n} \langle n^0 | m^0 \rangle \frac{\langle m^0 | H^1 | n^0 \rangle}{E_n^0 - E_m^0} \\
&= \langle n^0 | H^1 | n^1 \rangle \\
&= \langle n^0 | H^1 | \sum_{m \neq n} \frac{\langle m^0 | H^1 | n^0 \rangle}{E_n^0 - E_m^0} | m^0 \rangle \\
&= \sum_{m \neq n} \frac{|\langle m^0 | H^1 | n^0 \rangle|^2}{E_n^0 - E_m^0}.
\end{aligned}
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Check the example (6.1) in Griffiths.