Time-independent perturbation theory: degenerate case

So far we consider the situation when
\[ E_n \neq E_m \text{ for any } n \neq m \]
\[ |n> = \sum_{m \neq n} \frac{V_{mn}}{E_n - E_m} |m(0)> + |n(0)> \]

In many physical situations, \( E_n \) can be \( g \)-times degenerate in the absence of perturbation.

\[ \hat{H}_0 |m_D> = E_D |m_D> \]
\[ D = \{ |m_D> \} \quad \text{substate of} \quad g \quad \text{degenerate states} \]

It is important to note that any linear combination of \(|m_D>\) is an eigenstate, no preferred combination.

However, when we apply a perturbation, we still must require that it does not change the system substantially \(\Rightarrow\) necessary to find the basis in which is true.

Before \[ - - - \]
After \[ - - - \]
\[ \Rightarrow \quad \text{need to identify this basis} \]

First order correction in energy requires only zero-order wave functions.

Let \( |m_D> \in D \)
\[ \hat{H}_0 |m_D> = E_D^{(0)} |m_D> \]
\[ |m_D> = \sum_{m \in D} \langle m_D|m_D> \]
\[ |m_D> - \text{desired basis} \]
\[ |m_D> - \text{given basis} \]

\[ \hat{V}|m_D> = E_D^{(1)} |m_D> \]
\[ (E_D^{(1)} + \hat{V})|m_D> = 0 \]
Thus \( \hat{V} \) must be diagonal \( \hat{V} |n_p\rangle = V_{nn} |n_p\rangle \)
then \( E_{Dn}^{(1)} = V_{nn} \) - problem solved!

To figure out how to write \( \pi |n_p\rangle \) in terms of the original basis we need
to find \( \langle m_D | n_p \rangle = c_{mn} \)
\( \hat{V} |n_p\rangle = E_{Dn}^{(1)} |n_p\rangle \)
\( \sum_{mD} c_{mn} \hat{V} |m_D\rangle = E_{Dn}^{(1)} \sum_{mD} c_{mn} |m_D\rangle \)
\( \sum_{mD} c_{mn} \langle m_D | \hat{V} |m_D\rangle = \sum_{mD} E_{Dn}^{(1)} c_{mn} \langle m_D | m_D\rangle \)
\( \sum_{mD} c_{mn} (\langle m_D | \hat{V} |m_D\rangle - E_{Dn}^{(1)} \delta_{mm}) = 0 \)

\[ \text{det} [\hat{V} - E_{Dn}^{(1)} \mathbb{I}] = 0 \] (secular eqn)

In general, this equation will provide 9 separate solutions \( E_{Dn}^{(1)} \)
each \( E_{Dn}^{(1)} \) will correspond to the set of \( \{ c_{mn} \} \) to figure out a corresponding eigenstate in the subset \( D \).

Now when we identified the right basis, \( \pi |n_p\rangle \),
we can proceed with the calculations of the higher order corrections.

Assume the unperturbed system is in the state \( |k^{(0)}\rangle \in D \), \( |k^{(0)}\rangle \) is one of the \( \{ |n_p^{(0)}\rangle \} \) states

Solving for \( \hat{H} |k\rangle = (\hat{H}_0 + \hat{V}) |k\rangle = E_k |k\rangle \)
\[ |k\rangle = |k^{(0)}\rangle + \sum_{n_D \in D \not= k} c_{n_Dn_p}^{(1)} |n_D^{(0)}\rangle + \sum_{m_D \in D} c_{k_m}^{(1)} |m_D^{(0)}\rangle \]

\[ E_k^{(1)} = \langle k^{(0)} | \hat{V} |k^{(0)}\rangle = V_{kk} \]
\[ \hat{\mathcal{H}}_{0}|k^{(1)}\rangle + \hat{V}|k^{(0)}\rangle = E_{k}^{(0)}|k^{(1)}\rangle + E_{k}^{(1)}|k^{(0)}\rangle \]

for \( |m^{(0)}\rangle \notin \mathcal{D} \)

\[ \langle m^{(0)}|\hat{\mathcal{H}}_{0}|k^{(1)}\rangle + \langle m^{(0)}|\hat{V}|k^{(0)}\rangle = E_{k}^{(0)}\langle m^{(0)}|k^{(1)}\rangle + E_{k}^{(1)}\langle m^{(0)}|k^{(0)}\rangle \]

\[ E_{m}^{(0)}\langle m^{(0)}|k^{(1)}\rangle + V_{mk} = E_{k}^{(0)}\langle m^{(0)}|k^{(0)}\rangle \]

\[ \langle m^{(0)}|k^{(0)}\rangle = c_{km}^{(1)} = \frac{V_{mk}}{E_{k}^{(0)} - E_{m}^{(0)}} \]

\[ \text{just like before} \]

\[ \text{for } |n^{(0)}\rangle \notin \mathcal{D} \quad \text{(but } |n^{(0)}\rangle \neq |k^{(0)}\rangle) \]

\[ \langle n^{(0)}|\hat{\mathcal{H}}_{0}|k^{(1)}\rangle + \langle n^{(0)}|\hat{V}|k^{(0)}\rangle = E_{k}^{(0)}\langle n^{(0)}|k^{(1)}\rangle + E_{k}^{(1)}\langle n^{(0)}|k^{(0)}\rangle \]

\[ 0 = 0 \Rightarrow a_{mk}^{(1)} = 0 \]

\[ E_{k}^{(2)} = \langle k^{(0)}|\hat{V}|k^{(1)}\rangle = \langle k^{(0)}|\hat{V} \times \hat{\mathcal{S}}|k^{(0)}\rangle + \sum_{m \notin \mathcal{D}} \frac{V_{mk}}{E_{k}^{(0)} - E_{m}^{(0)}} \]

\[ = V_{kk} + \sum_{m \notin \mathcal{D}} \frac{V_{mk}k^{2}}{E_{k}^{(0)} - E_{m}^{(0)}} \]

\[ \text{Formally identical to the undegenerate PT} \]

One can show that the first not vanishing contributions from \( |n^{(0)}\rangle \neq |k^{(0)}\rangle \) comes in the second order wave-function corrections.

\[ e_{mk}^{(2)} = \frac{1}{V_{kk} - V_{Hmk}} \sum_{m \notin \mathcal{D}} \frac{V_{mk}}{E_{k}^{(0)} - E_{m}^{(0)}} \]
Our goal is to investigate the atomic structure, but let's look for a moment on a two-level system.

(Example: quantization of electron rotation)

\[ E_{\text{kin}} = \frac{\hbar^2 k^2}{2m} + \frac{eB}{mc}(n+\frac{1}{2}) \]

If we at \( B_0 \), two states (e.g., \( |0\rangle \) and \( |1\rangle \)) have the same energy \( E_0 \).

Turn on the perturbation

\[ \hat{V} = \begin{pmatrix} V_{00} & V_{01} \\ V_{10} & V_{11} \end{pmatrix} \quad \Delta E \quad \text{first-order correction} \]

Looking for a "correct" basis

\[ |d\rangle = c_0 |0\rangle + c_1 |1\rangle \]

Secular equation

\[ \det \begin{vmatrix} V_{00} - \Delta E & V_{01} \\ V_{10} & V_{11} - \Delta E \end{vmatrix} = 0 \]

\[ \Delta E^2 - (V_{00}+V_{11})\Delta E + V_{00}V_{11} - |V_{01}|^2 = 0 \]

\[ \Delta E = \frac{V_{00}+V_{11}}{2} \pm \frac{\sqrt{(V_{00}-V_{11})^2 + 4|V_{01}|^2}}{2} \]
To simplify the math a little, let's assume that $V_{00} = V_{11} = 0$ (i.e., our original basis is really wrong!)

$$V = \begin{pmatrix} 0 & V \\ V^* & 0 \end{pmatrix}$$

$$\Delta E_{1,2} = \pm |V|$$

Degeneracy is lifted

Assume $V$ to be real and positive

$$\Delta E = V \begin{pmatrix} -V \\ V \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = 0 \Rightarrow c_0 = c_1$$

$$|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle + |1\rangle)$$

$$\Delta E = -V \begin{pmatrix} V \\ V \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} \Rightarrow c_0 = -c_1$$

$$|1\rangle = \frac{1}{\sqrt{2}} (|0\rangle - |1\rangle)$$

State = $|1\rangle$

10\rangle level crossing

Avoided crossing