Time-independent perturbation theory: degenerate case

So far we consider the situation when

$E_n \neq E_m$ for any $n \neq m$

$$|n\rangle = |n^{(0)}\rangle + \lambda \sum_{m \neq n} |m^{(0)}\rangle \frac{V_{mn}}{E_n^{(0)} - E_m^{(0)}}$$

In many physical situations E_n can be g-times degenerate in the absence of perturbation

$$\hat{H}_0 |m_D\rangle = E_D |m_D\rangle \qquad D \equiv \{|m_D\rangle\}$$ substate of g degenerate states

It is important to note that any lin. combination of $|m_D\rangle$ is an eigenstate, no preferred combination.

However, when we apply a perturbation, we still must require that it does not change the system substantially => necessary to find the basis in which is true!

before after

need to identify this basis

First order correction in energy requires only zero-order wavefunctions

Let $|n_D\rangle \in D \qquad \hat{H}_0 |n_D\rangle = E_D^{(0)} |n_D\rangle$

$$|n_D\rangle = \sum_{m \in D} |m_D\rangle \langle m_D | n_D\rangle$$

$|n_D\rangle$ - desired basis

$|m_D\rangle$ - given basis

$$\hat{H} |n_D\rangle = (\cancel{\hat{H}_0} + \lambda \hat{V}) |n_D\rangle = (\cancel{E_D} + \lambda E_{Dn}^{(1)}) |n_D\rangle$$

$$\hat{V} |n_D\rangle = E_{Dn}^{(1)} |n_D\rangle$$

$$(E_{Dn}^{(1)} - \hat{V}) |n_D\rangle = 0$$

Thus $\hat{V}$ must be diagonal $\hat{V}|n_D\rangle = V_{nn}|n_D\rangle$

then $E^{(1)}_{Dn} = V_{nn}$ – problem solved!

To figure out how to write $\{|n_D\rangle\}$ in terms of the original basis we need to find $\langle m_D|n_D\rangle = c_{mn}$

$$\hat{V}|n_D\rangle = E^{(1)}_{Dn}|n_D\rangle$$

$$\sum_{m\in D} c_{mn}\hat{V}|m_D\rangle = E^{(1)}_{Dn}\sum_{m\in D} c_{mn}|m_D\rangle$$

$$\sum_{m\in D} c_{mn}\langle m'_D|\hat{V}|m_D\rangle = \sum_{m\in D} E^{(1)}_{Dn} c_{mn}\overbrace{\langle m'_D|m_D\rangle}^{\delta_{mm'}}$$

$$\sum_{m\in D} c_{mn}\left(\langle m'_D|V|m_D\rangle - E^{(1)}_{Dn}\delta_{mm'}\right) = 0$$

$$\det\left[\hat{V} - E^{(1)}_{Dn}\hat{I}\right] = 0 \qquad \text{(secular eqn)}$$

In general, this equation will provide g separate solutions $E^{(1)}_{Dn}$

each $E^{(1)}_{Dn}$ 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, $\{|n_D\rangle\}$, 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 $\{|n^{(0)}_D\rangle\}$ states

Solving for $\hat{H}|k\rangle = (\hat{H}_0 + \lambda\hat{V})|k\rangle = E_k|k\rangle$

$$|k\rangle = |k^{(0)}\rangle + \underbrace{\lambda\sum_{\substack{n_D\in D\\ n_D\neq k}} c^{(1)}_{kn_D}|n^{(0)}_D\rangle + \lambda\sum_{m\notin D} c^{(1)}_{km}|m\rangle}_{|k^{(1)}\rangle}$$

$$E^{(1)}_k = \langle k^{(0)}|V|k^{(0)}\rangle = V_{kk}$$

$$\hat{H}_0 |k^{(1)}\rangle + \hat{V}|k^{(0)}\rangle = E_k^{(0)} |k^{(1)}\rangle + E_k^{(1)} |k^{(0)}\rangle$$

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

$$\langle m^{(0)}|\hat{H}_0|k^{(1)}\rangle + \langle m^{(0)}|\hat{V}|k^{(0)}\rangle = E_k^{(0)} |k^{(1)}\rangle + \underbrace{E_k^{(1)} \langle m|k^{(0)}\rangle}_{=0}$$

$$E_m^{(0)} \langle m^{(0)}|k^{(1)}\rangle + V_{mk} = E_k^{(0)} \langle m^{(0)}|k^{(0)}\rangle$$

$$\langle m^{(0)}|k^{(1)}\rangle = c_{km}^{(1)} = V_{mk} / (E_k^{(0)} - E_n^{(0)})$$ just like before

for $|n_D\rangle \in D$ (but $|n_D\rangle \neq |k\rangle$)

$$\langle n_D^{(0)}|\hat{H}_0|k^{(1)}\rangle + \langle n_D|\hat{V}|k^{(0)}\rangle = E_k^{(0)} \langle n_D|k^{(1)}\rangle + E_k^{(1)} \langle n_D|k^{(0)}\rangle$$

$$0 = 0 \quad \Rightarrow \quad c_{n_D k}^{(1)} = 0$$

$$E_k^{(2)} = \langle k^{(0)}|\hat{V}|k^{(1)}\rangle = \langle k^{(0)}|\hat{V} \times \left\{ |k^{(0)}\rangle + \sum_{m \notin D} \frac{V_{mk}}{E_k^{(0)} - E_m^{(0)}} |m^{(0)}\rangle \right\}$$

$$= V_{kk} + \sum_{m \notin D} \frac{|V_{mk}|^2}{E_k^{(0)} - E_m^{(0)}}$$

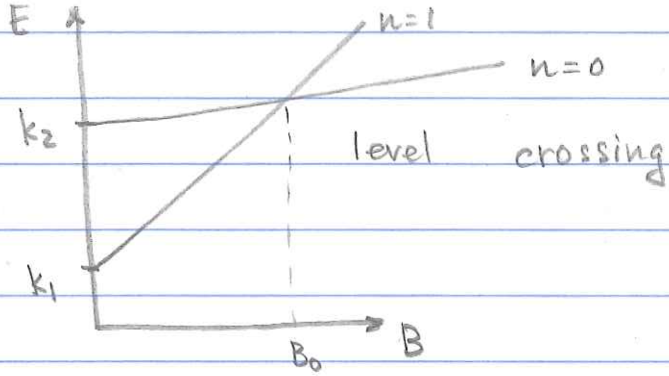
Formally identical to the undegenerate PT

One can show that the first not vanishing contributions from $\{|n_D\rangle\} \neq k$ comes in the second order wave-function corrections

$$c_{n_D k}^{(2)} = \frac{1}{V_{kk} - V_{n_D n_D}} \sum_{m \notin D} \frac{V_{n_D m} V_{mk}}{E_k^{(0)} - E_m^{(0)}}$$

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)

$$E_{k,n} = \frac{\hbar^2 k^2}{2m} + \frac{e\hbar}{mc} B \left(n+\frac{1}{2}\right)$$



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

Turn on the perturbation

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

Looking for a "correct" basis

$|\alpha\rangle = c_0|0\rangle + c_1|1\rangle$

Secular equation $\det \begin{vmatrix} V_{00}-\Delta E & V_{01} \\ V_{10} & V_{11}-\Delta E \end{vmatrix} = 0$

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

$$\Delta E_{1,2} = \frac{V_{00}+V_{11}}{2} \pm \frac{\sqrt{(V_{00}-V_{11})^2 + 4|V_{01}|^2}}{2}$$

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

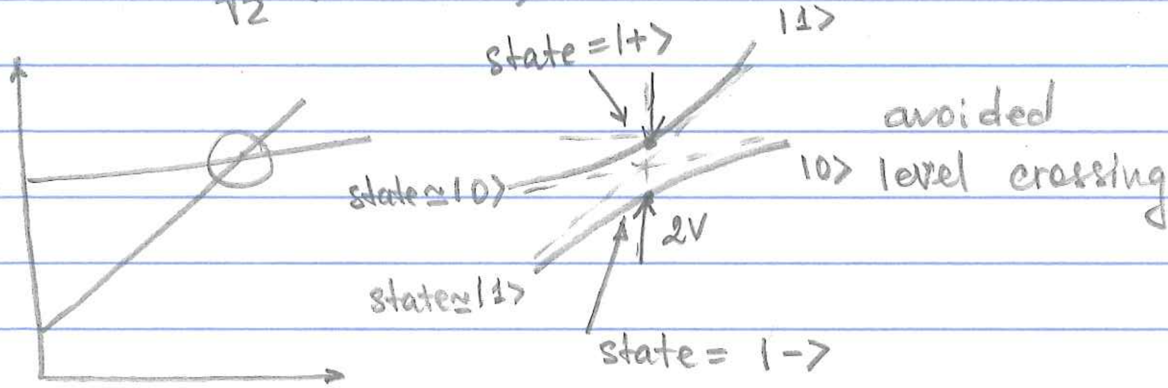
Assume V to be real and positive

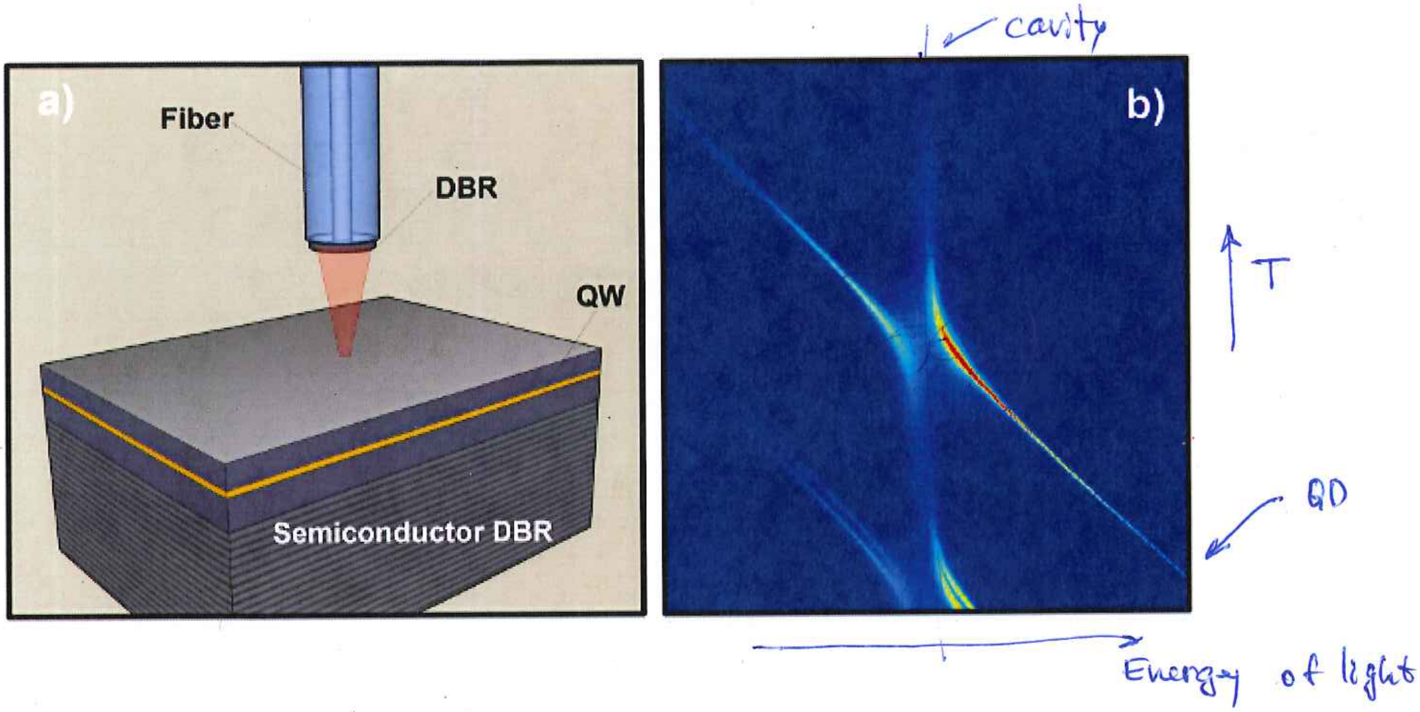
$$\Delta E = V \qquad \begin{pmatrix} -V & V \\ V & -V \end{pmatrix} \begin{pmatrix} c_0 \\ c_1 \end{pmatrix} = 0 \qquad \Rightarrow \quad c_0 = c_1$$

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

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

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




a)
Fiber
DBR
QW
Semiconductor DBR
b)
cavity
T
QD
Energy of light