

February 26, 2016

Time Independent Perturbation Theory

$$i\hbar \frac{\partial \psi}{\partial t} = H \psi \quad E \psi = H \psi$$

$$H = H^0 + H'$$

$$H^0 \psi_n^0 = E_n^0 \psi_n^0$$

$\{E_n^0\}$ eigenvalues of H^0
 $\{\psi_n^0\}$ eigenfunctions of H^0

$$H_\lambda = H^0 + \lambda H'$$

$$H = H_\lambda$$

$$H_\lambda \psi_n(\vec{r}; \lambda) = E_n(\lambda) \psi_n(\vec{r}, \lambda)$$

$$E_n(\lambda) = E_n^0 + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$

$$\psi_n(\vec{r}; \lambda) = \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \dots$$

$$\begin{aligned} (H^0 + \lambda H') (\psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + O(\lambda^3)) \\ = (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + O(\lambda^3)) (\psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + O(\lambda^3)) \end{aligned}$$

$$\lambda^0 : H^0 \psi_n^{(0)} = E_n^{(0)} \psi_n^{(0)}$$

$$\lambda^1 : H^0 \psi_n^{(1)} + H' \psi_n^{(0)} = E_n^{(0)} \psi_n^{(1)} + E_n^{(1)} \psi_n^{(0)}$$

$$H^0 |n\rangle^{(0)} = E_n^{(0)} |n\rangle^{(0)}$$

$$\langle n | (H^0 |n\rangle^{(1)} + H' |n\rangle^{(0)}) = E_n^{(0)} |n\rangle^{(1)} + E_n^{(1)} |n\rangle^{(0)}$$

$$E_n^{(0)} \langle n | n \rangle^{(0)} + \langle n | H' |n\rangle^{(0)} = E_n^{(0)} \langle n | n \rangle^{(0)} + E_n^{(1)}$$

$$E_n^{(1)} = \langle n | H' |n\rangle^{(0)} = \int d^3r \psi_n^{*(0)}(\vec{r}) H' \psi_n^{(0)}(\vec{r})$$

$$(H^{(0)} - E_n^{(0)}) \psi_n^{(1)} = (E_n^{(1)} - H') \psi_n^{(0)}$$

$$|n\rangle^{(1)} = \sum a_{nm} |m\rangle^{(0)}$$

$$\langle k | \left[\sum a_{nm} (E_m^{(0)} - E_n^{(0)}) |m\rangle^{(0)} \right] = \left[(E_n^{(1)} - H') |n\rangle^{(0)} \right]$$

$\{|m\rangle^{(0)}\}$ is an orthonormal basis

$$a_{nk} (E_k^{(0)} - E_n^{(0)}) = \langle k | E_n^{(1)} - H' |n\rangle^{(0)}$$

$$a_{nk} = \frac{E_n^{(1)} \delta_{kn} - \langle k | H' |n\rangle^{(0)}}{E_k^{(0)} - E_n^{(0)}} \quad \text{if } E_k^{(0)} - E_n^{(0)} \neq 0$$

$$a_{nk} = - \frac{\langle k | H' |n\rangle^{(0)}}{E_k^{(0)} - E_n^{(0)}} = \frac{\langle k | H' |n\rangle^{(0)}}{E_n^{(0)} - E_k^{(0)}} \quad (\text{if } n \neq k)$$

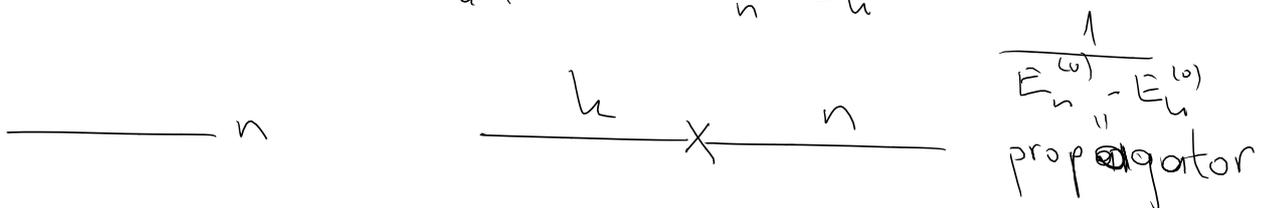
if the spectrum is not degenerate, then
 $n \neq k \Rightarrow E_n^{(0)} \neq E_k^{(0)}$

$$|n\rangle^{(1)} = \frac{a_{nn} |n\rangle^{(0)}}{1} + \sum_{k \neq n} \frac{\langle k | H' |n\rangle^{(0)}}{E_n^{(0)} - E_k^{(0)}} |k\rangle^{(0)}$$

choose $a_{nn} = 0$

$$|n\rangle^{(1)} = \sum_{k \neq n} \frac{\langle k | H' |n\rangle^{(0)}}{E_n^{(0)} - E_k^{(0)}} |k\rangle^{(0)}$$

$$|n\rangle = \underbrace{|n\rangle^{(0)}}_n + \sum_{k \neq n} |k\rangle^{(0)} \frac{1}{E_n^{(0)} - E_k^{(0)}} \langle k | H' |n\rangle^{(0)} + \dots$$



$$\frac{1}{h'} + \frac{1}{h} = \frac{h + h'}{hh'}$$

$$| \psi_n^{(2)} \rangle = \sum_{k \neq n} \frac{1}{h'k} |k\rangle \frac{1}{E_k^{(0)} - E_n^{(0)}} \langle k | H' | k \rangle \frac{1}{E_n^{(0)} - E_n^{(0)}} \langle k | H' | n \rangle$$

$$\hat{\lambda}^2 : H^0 \psi_n^{(2)} + H' \psi_n^{(1)} = E_n^{(2)} \psi_n^{(0)} + E_n^{(1)} \psi_n^{(1)} + E_n^{(0)} \psi_n^{(2)}$$

$$\langle n | (H^0 |n\rangle^{(2)} + H' |n\rangle^{(2)}) = E_n^{(2)} \langle n | n \rangle^{(0)} + E_n^{(1)} \langle n | n \rangle^{(1)} + E_n^{(0)} \langle n | n \rangle^{(2)}$$

$$\langle n | H' | n \rangle^{(2)} = E_n^{(2)} + E_n^{(1)} \langle n | n \rangle^{(0)}$$

$$E_n^{(2)} = - \langle n | H' | n \rangle^{(2)} + E_n^{(1)} \langle n | n \rangle^{(1)}$$

$$E_n^{(2)} = - \langle n | H' | n \rangle^{(2)}$$

$$E_n^{(2)} = - \sum_{k \neq n} \frac{|\langle n | H' | k \rangle^{(0)}|^2}{E_n^{(0)} - E_k^{(0)}}$$

since $\langle n | n \rangle^{(1)} = \langle n | n \rangle = 0$

$$E_n^{(2)} = \langle \psi_n | H | \psi_n \rangle$$

$$= \left(\langle n | + \lambda \langle n |^{(1)} + \lambda^2 \langle n |^{(2)} + \dots \right) (H^{(0)} + \lambda H')$$

$$\left(|n\rangle^{(0)} + \lambda |n\rangle^{(1)} + \lambda^2 |n\rangle^{(2)} + \dots \right)$$

$$E_n^{(0)} = \langle n | H^{(0)} | n \rangle^{(0)}$$

$$E_n^{(1)} = \langle n | H' | n \rangle^{(0)} + \langle n | H^{(0)} | n \rangle^{(1)}$$

$$H_\lambda |n\rangle = E_n^{(0)} |n\rangle$$

$$(H^{(0)} + \lambda H') |n\rangle = E_n |n\rangle$$

$$(H^{(0)} - E_n^{(0)}) |n\rangle = (\lambda H' + \Delta E_n) |n\rangle$$

$$\begin{aligned} |n\rangle &= |n\rangle^0 + \frac{1}{H^{(0)} - E_n^{(0)}} (\lambda H' + \Delta E_n) |n\rangle \\ &= |n\rangle^0 + \lambda \frac{1}{H^{(0)} - E_n^{(0)}} \tilde{H} |n\rangle^0 + \lambda^2 \frac{1}{H^{(0)} - E_n^{(0)}} \tilde{H} \frac{1}{H^{(0)} - E_n^{(0)}} |n\rangle \end{aligned}$$

$$\begin{aligned} \frac{1}{H^{(0)} - E_n^{(0)}} \tilde{H} |n\rangle^{(0)} &= \sum_m |m\rangle^0 \langle m| \frac{1}{H^{(0)} - E_n^{(0)}} H' |n\rangle^{(0)} \\ &= \sum_m |n\rangle^0 \langle m| H' |n\rangle^{(0)} \frac{1}{E_n^{(0)} - E_m^{(0)}} \end{aligned}$$

Degenerate Perturbation Theory

$$H_\lambda = H_0 + \lambda H'$$

$$|n\rangle = \underline{|n\rangle^{(0)}} + \lambda |n\rangle^{(1)} + \lambda^2 |n\rangle^{(2)} + \dots$$

Assume

$|n\rangle^{(0)}$ and $|n'\rangle^{(0)}$ are degenerate.

$$|n\rangle = \alpha |n\rangle^{(0)} + \beta |n'\rangle^{(0)} + \mathcal{O}(\lambda)$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)}$$

$$H^0 |n\rangle^{(0)} = E_n^{(0)} |n\rangle^{(0)}$$

$$H^0 |n'\rangle^{(0)} = E_n^{(0)} |n'\rangle^{(0)}$$

$$\begin{aligned}
 & (H^{(0)} + \lambda H') (\alpha |n\rangle^{(0)} + \beta |n'\rangle^{(0)} + \lambda |n\rangle^{(1)} + O(\lambda^2)) \\
 \langle n|, \langle n'| & = (E_n^{(0)} + \lambda E_n^{(1)} + O(\lambda^2)) (\alpha |n\rangle^{(0)} + \beta |n'\rangle^{(0)} + \lambda |n\rangle^{(1)}) \\
 \lambda^{-1} : & \left[H^{(0)} |n\rangle^{(1)} + H' (\alpha |n\rangle^{(0)} + \beta |n'\rangle^{(0)}) \right. \\
 & \left. = E_n^{(0)} |n\rangle^{(1)} + E_n^{(1)} (\alpha |n\rangle^{(0)} + \beta |n'\rangle^{(0)}) \right]
 \end{aligned}$$

$$\begin{aligned}
 \alpha \langle n| H' |n\rangle^{(0)} + \beta \langle n| H' |n'\rangle^{(0)} \\
 = E_n^{(1)} \alpha
 \end{aligned}$$

$$\begin{aligned}
 \alpha \langle n'| H' |n\rangle^{(0)} + \beta \langle n'| H' |n'\rangle^{(0)} \\
 = E_n^{(1)} \beta
 \end{aligned}$$

$$\begin{pmatrix} \langle n| H' |n\rangle^{(0)} & \langle n| H' |n'\rangle^{(0)} \\ \langle n'| H' |n\rangle^{(0)} & \langle n'| H' |n'\rangle^{(0)} \end{pmatrix} \begin{pmatrix} \alpha \\ \beta \end{pmatrix} = E_n^{(1)} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}$$

Nontrivial Soln. Exists only if

$$\det \begin{pmatrix} H'_{nn} & H'_{nn'} \\ H'_{n'n} & H'_{n'n'} \end{pmatrix} - E_n^{(1)} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = 0$$

$$\det \begin{pmatrix} H'_{nn} - E_n^{(1)} & H'_{nn'} \\ H'_{n'n} & H'_{n'n'} - E_n^{(1)} \end{pmatrix} = (H'_{nn} - E_n^{(1)}) (H'_{n'n'} - E_n^{(1)}) - H'_{n'n} H'_{nn'} = 0$$

$$E_n^{(1)} = a + b \quad \text{or} \quad E_n^{(1)} = a - b$$

Example

$$H^0 = \begin{pmatrix} \varepsilon & 0 \\ 0 & \varepsilon \end{pmatrix}, \quad H' = \begin{pmatrix} 0 & \delta \\ \delta & 0 \end{pmatrix}$$

$$H = \begin{pmatrix} \varepsilon & \delta \\ \delta & \varepsilon \end{pmatrix}$$

$$H \begin{pmatrix} 1 \\ 1 \end{pmatrix} \frac{1}{\sqrt{2}} = (\varepsilon + \delta) \begin{pmatrix} 1/\sqrt{2} \\ 1/\sqrt{2} \end{pmatrix}$$

$$H \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix} = (\varepsilon - \delta) \begin{pmatrix} 1/\sqrt{2} \\ -1/\sqrt{2} \end{pmatrix}$$

$$| \psi \rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad | \psi' \rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} H'_{11} & H'_{11'} \\ H'_{11'} & H'_{11'} \end{pmatrix} = \begin{pmatrix} 0 & \delta \\ \delta & 0 \end{pmatrix}$$

To determine $E_n^{(2)}$

$$\det \begin{pmatrix} -E_n^{(2)} & \delta \\ \delta & -E_n^{(2)} \end{pmatrix} = \left(E_n^{(2)} \right)^2 - \delta^2 = 0$$

$$\Rightarrow E_n^{(2)} = \delta \quad \text{or} \quad E_n^{(2)} = -\delta$$

$$\begin{pmatrix} 0 & \delta \\ \delta & 0 \end{pmatrix} \begin{pmatrix} \alpha_{\pm} \\ \beta_{\pm} \end{pmatrix} = \pm \delta \begin{pmatrix} \alpha_{\pm} \\ \beta_{\pm} \end{pmatrix}$$

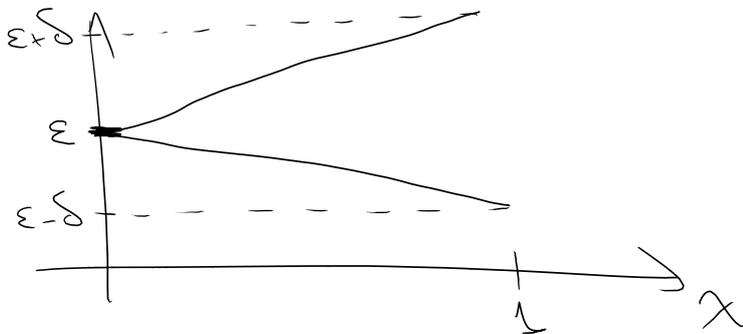
$$\begin{pmatrix} \beta_{\pm} \delta \\ \alpha_{\pm} \delta \end{pmatrix} = \begin{pmatrix} \pm \delta \alpha_{\pm} \\ \pm \delta \beta_{\pm} \end{pmatrix}$$

$$\beta_{\pm} \cancel{\delta} = \pm \cancel{\delta} \alpha_{\pm}$$
$$\beta_{\pm} = \pm \alpha_{\pm}$$

$$\beta_{+} = \alpha_{+}; \quad \beta_{-} = -\alpha_{-}$$

$$+\delta : \begin{pmatrix} \alpha_+ \\ \beta_+ \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} \end{pmatrix}$$

$$-\delta : \begin{pmatrix} \alpha_- \\ \beta_- \end{pmatrix} = \begin{pmatrix} \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} \end{pmatrix}$$



Example

$$H' = \begin{pmatrix} 0 & \delta \\ \delta & 0 \end{pmatrix}; H^0 = \begin{pmatrix} \epsilon_1 & 0 \\ 0 & \epsilon_2 \end{pmatrix}$$

$$|1\rangle \equiv \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$|2\rangle \equiv \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$H^0 |1\rangle^{(0)} = \epsilon_1 |1\rangle^{(0)}; H^0 |2\rangle^{(0)} = \epsilon_2 |2\rangle^{(0)}$$

$$E_1^{(1)} = \langle 1 | H' | 1 \rangle^{(0)} = 0$$

$$E_2^{(1)} = \langle 2 | H' | 2 \rangle^{(0)} = 0$$

$$|1\rangle^{(1)} = \frac{\langle 2 | H' | 1 \rangle^{(0)} |2\rangle^{(0)}}{\epsilon_1 - \epsilon_2} = \frac{\delta}{\epsilon_1 - \epsilon_2} |2\rangle^{(0)}$$

$$|2\rangle^{(1)} = \frac{\langle 1 | H' | 2 \rangle^{(0)} |1\rangle^{(0)}}{\epsilon_2 - \epsilon_1} = \frac{\delta}{\epsilon_2 - \epsilon_1} |1\rangle^{(0)}$$

$$|1\rangle = |1\rangle^{(0)} + \frac{\delta}{\epsilon_1 - \epsilon_2} |2\rangle^{(0)} + \dots$$

$$|2\rangle = |2\rangle^{(0)} - \frac{\delta}{\epsilon_1 - \epsilon_2} |1\rangle^{(0)} + \dots$$

$$E_1^{(2)} = - \frac{|\langle 2 | H' | 1 \rangle|^2}{\epsilon_1 - \epsilon_2} = - \frac{\delta^2}{\epsilon_2 - \epsilon_1}$$

$$E_2^{(2)} = - \frac{|\langle 1 | H' | 2 \rangle|^2}{\epsilon_2 - \epsilon_1} = - \frac{\delta^2}{\epsilon_2 - \epsilon_1}$$

Exact soln

$$H = \begin{pmatrix} \epsilon_1 & \delta \\ \delta & \epsilon_2 \end{pmatrix} \quad \det(H - \epsilon \mathbb{1}) = 0$$

$$(\epsilon_1 - \epsilon)(\epsilon_2 - \epsilon) - \delta^2 = 0$$

$$\epsilon^2 - (\epsilon_1 + \epsilon_2)\epsilon + (\epsilon_1\epsilon_2 - \delta^2) = 0$$

$$\epsilon = \frac{\epsilon_1 + \epsilon_2 \pm \sqrt{(\epsilon_1 + \epsilon_2)^2 - 4(\epsilon_1\epsilon_2 - \delta^2)}}{2}$$

$$\epsilon = \left[\epsilon_1 + \epsilon_2 \pm |\epsilon_1 - \epsilon_2| \sqrt{1 + \frac{4\delta^2}{(\epsilon_1 - \epsilon_2)^2}} \right] \frac{1}{2}$$

$$|1\rangle = \cos\theta |1\rangle^{(0)} + \sin\theta |2\rangle^{(0)}$$

$$|2\rangle = -\sin\theta |1\rangle^{(0)} + \cos\theta |2\rangle^{(0)}$$

$$\langle 2 | H | 1 \rangle = 0 \Rightarrow -\sin\theta \cos\theta \epsilon_1 + \sin\theta \cos\theta \epsilon_2 - \sin^2\theta \delta + \cos^2\theta \delta$$

$$\sin\theta \cos\theta (\epsilon_2 - \epsilon_1) + (\cos^2\theta - \sin^2\theta) \delta = 0$$

$$\frac{1}{2} \sin 2\theta (\epsilon_2 - \epsilon_1) + \cos 2\theta \delta = 0$$

$$\boxed{\tan 2\theta = \frac{2\delta}{\epsilon_1 - \epsilon_2}}$$

$$\text{if } \theta \ll 1 \quad \tan 2\theta \approx 2\theta \Rightarrow \theta = \frac{\delta}{\epsilon_1 - \epsilon_2}$$