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the first order correction to the wavefunction

$$\langle k|② = \sum_n c_n \langle k|[E_n^{(0)}-E_0^{(0)}]|n\rangle = \langle k|[E_0^{(1)}-H^{(1)}]|0\rangle$$

$$c_k[E_k^{(0)}-E_0^{(0)}] = E_0^{(1)}\langle k|0\rangle - \langle k|H^{(1)}|0\rangle = -\langle k|H^{(1)}|0\rangle$$

$$c_k = \frac{H_{k0}^{(1)}}{E_0^{(0)}-E_k^{(0)}}$$

$$\psi_0 \approx \psi_0^{(0)} + \sum_{k\neq 0}\frac{H_{k0}^{(1)}}{E_0^{(0)}-E_k^{(0)}}\psi_k^{(0)}$$

Ex: for previous example

$n=2 \quad H_{21}^{(1)}=0 \quad c_2=0$

$$c_3 = \frac{\int_0^L \psi_3^* H^{(1)}\psi_1\,dx}{E_1^{(0)}-E_3^{(0)}} = \frac{\varepsilon\frac{2}{L}\int_{\frac{1}{2}(L-a)}^{\frac{1}{2}(L+a)}\sin(\frac{3\pi x}{L})\sin(\frac{\pi x}{L})dx}{\frac{\hbar^2}{8mL^2}-\frac{9\hbar^2}{8mL^2}}$$

$$= \frac{\varepsilon\frac{2}{L}}{-\frac{\hbar^2}{mL^2}}\left[\frac{\sin(\frac{11\pi}{10})}{\frac{4\pi}{L}} - \frac{\sin(\frac{11\pi}{5})}{\frac{8\pi}{L}} - \frac{\sin(\frac{9\pi}{10})}{\frac{4\pi}{L}} - \frac{\sin(\frac{9\pi}{5})}{\frac{8\pi}{L}}\right]$$

$$= 0.192\frac{\varepsilon}{\frac{\hbar^2}{mL^2}}$$

$$\Rightarrow \psi_1 = \psi_1^{(0)} + 0.192\frac{\varepsilon mL^2}{\hbar^2}\psi_3^{(0)}$$

the second order correction to the energy

$$\psi_0^{(2)} = \sum_n b_n \psi_n^{(0)}$$

$$\Rightarrow \sum_n b_n[E_n^{(0)}-E_0^{(0)}]|n\rangle = [E_0^{(2)}-H^{(2)}]|0\rangle + \sum_n c_n[E_0^{(1)}-H^{(1)}]|n\rangle \;\times\langle 0|$$

$$\sum_n b_n[E_n^{(0)}-E_0^{(0)}]\langle 0|n\rangle = \langle 0|[E_0^{(2)}-H^{(2)}]|0\rangle + \sum_n c_n\langle 0|[E_0^{(1)}-H^{(1)}]|n\rangle$$

$$= E_0^{(2)} - \langle 0|H^{(2)}|0\rangle + \sum_n c_n\langle 0|[E_0^{(1)}-H^{(1)}]|n\rangle$$

$$0 = E_0^{(2)} - \langle 0|H^{(2)}|0\rangle + c_0[E_0^{(1)} - \langle 0|H^{(1)}|0\rangle] + \sum_{n\neq 0} c_n\langle 0|E_0^{(1)}-H^{(1)}|n\rangle$$

$$E_0^{(2)} = H_{00}^{(2)} + \sum_{n\neq 0}\frac{H_{0n}^{(1)}H_{n0}^{(1)}}{E_0^{(0)}-E_n^{(0)}} \quad = H_{0n}^{(1)}H_{0n}^{(1)*} = |H_{0n}^{(1)}|^2$$

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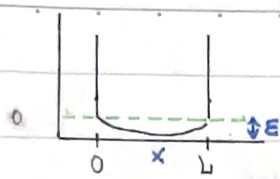
Ex:




$-\varepsilon\sin(\frac{\pi x}{L})$

find second order
$n=1$

$$H'_{n1} = -\frac{2\varepsilon}{L}\int_0^L \sin(\frac{n\pi x}{L})\sin(\frac{\pi x}{L})\sin(\frac{\pi x}{L})dx$$

$$= \frac{\varepsilon}{\pi}\left[\frac{1}{n}-\frac{1}{2(n+2)}-\frac{1}{2(n-2)}\right]\left[(-1)^n-1\right]$$

$$E_1^{(2)} = \frac{32mL^2\varepsilon^2}{h^2\pi^2}\sum_{n=3,5,\cdots}\frac{1}{1-n^2}\left[\frac{1}{n}-\frac{1}{2(n+2)}-\frac{1}{2(n-2)}\right]^2 = -\frac{32mL^2\varepsilon^2}{h^2\pi^2}\ 8.953\times10^{-3}$$

general

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

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

$$\hat{H}^0\psi_n^{(1)}-E_n^{(0)}\psi_n^{(1)} = E_n^{(1)}\psi_n^{(0)}-\hat{H}'\psi_n^{(0)} \quad \downarrow \times\psi_m^{(0)*}$$

$$\underline{\langle\psi_m^{(0)}|\hat{H}^0|\psi_n^{(1)}\rangle} - E_n\langle\psi_m^{(0)}|\psi_n^{(1)}\rangle = E_n^{(1)}\langle\psi_m^{(0)}|\psi_n^{(0)}\rangle - \langle\psi_m^{(0)}|\hat{H}'|\psi_n^{(0)}\rangle$$

$$= \langle\psi_n^{(1)}|\hat{H}^0|\psi_m^{(0)}\rangle^* = \langle\psi_n^{(1)}|E_m^{(0)}\psi_m^{(0)}\rangle^* = E_m^{(0)}\langle\psi_m^{(0)}|\psi_n^{(1)}\rangle$$

$$(E_m^{(0)}-E_n^{(0)})\langle\psi_m^{(0)}|\psi_n^{(1)}\rangle = E_n^{(1)}\delta_{mn}-\langle\psi_m^{(0)}|\hat{H}'|\psi_n^{(0)}\rangle$$

if $m=n$ $\quad E_n^{(1)} = \langle\psi_n^{(0)}|\hat{H}'|\psi_n^{(0)}\rangle = \int\psi_n^{(0)*}\hat{H}'\psi_n^{(0)}d\tau$

$$E_n \approx E_n^{(0)}+\lambda E_n^{(1)} = E_n^{(0)}+\int\psi_n^{(0)*}\hat{H}'\psi_n^{(0)}d\tau \quad \text{if } \lambda=1$$

if $m\neq n$ $\quad (E_m^{(0)}-E_n^{(0)})\underbrace{\langle\psi_m^{(0)}|\psi_n^{(1)}\rangle}_{a_m} = -\langle\psi_m^{(0)}|\hat{H}'|\psi_n^{(0)}\rangle$

$\psi_n^{(1)} = \sum_m a_m\psi_m^{(0)}$

$a_m = \langle\psi_m^{(0)}|\psi_n^{(1)}\rangle$

$$a_m = \frac{\langle\psi_m^{(0)}|\hat{H}'|\psi_n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}}$$

$$\psi_n \approx \psi_n^{(0)}+\sum_{m\neq n}\frac{\langle\psi_m^{(0)}|\hat{H}'|\psi_n^{(0)}\rangle}{E_n^{(0)}-E_m^{(0)}}\psi_m^{(0)}$$

similar, $\quad E_n^{(2)} = \sum_{m\neq n}\frac{|\langle\psi_m^{(0)}|\hat{H}'|\psi_n^{(0)}\rangle|^2}{E_n^{(0)}-E_m^{(0)}}$

$$E_n \approx E_n^{(0)}+E_n^{(1)}+\sum_{m\neq n}\frac{|H'_{mn}|^2}{E_n^{(0)}-E_m^{(0)}}$$

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