Perturbation Theory

Time-Independent

Nondegenerate for two level system

Consider first a system that has only two eigenstates

$$H^{(0)}\psi_m^{(0)} = E_m^{(0)}\psi_m^{(0)} \quad m=1,2 \qquad H\psi = E\psi$$

$$\psi = c_1\psi_1^{(0)} + c_2\psi_2^{(0)}$$

$$\Rightarrow H(c_1\psi_1^{(0)} + c_2\psi_2^{(0)}) = E(c_1\psi_1^{(0)} + c_2\psi_2^{(0)}), \quad c_1(H-E)|1\rangle + c_2(H-E)|2\rangle = 0 \;—\; ①$$

$$\left.\begin{aligned} \langle 1|① &= c_1(H_{11}-E) + c_2H_{12} = 0 \\ \langle 2|① &= c_1H_{21} + c_2(H_{22}-E) = 0 \end{aligned}\right\} \quad \begin{vmatrix} H_{11}-E & H_{12} \\ H_{21} & H_{22}-E \end{vmatrix} = 0$$

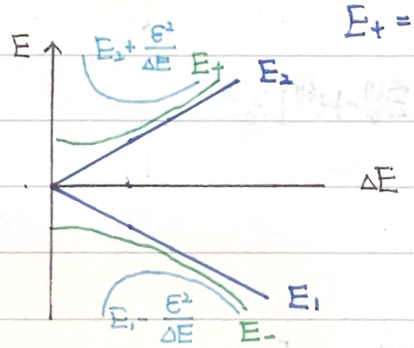
$$(H_{11}-E)(H_{22}-E) - H_{12}H_{21} = 0 = E^2 - (H_{11}+H_{22})E + H_{11}H_{22} - H_{12}H_{21} = 0$$

$$\Rightarrow E_\pm = \frac{1}{2}(H_{11}+H_{22}) \pm \frac{1}{2}\sqrt{(H_{22}-H_{11})^2 + 4H_{12}H_{21}}$$

$$= \frac{1}{2}(E_1^{(0)} + E_2^{(0)}) \pm \frac{1}{2}\sqrt{(E_2^{(0)} - E_1^{(0)})^2 + 4\varepsilon^2}$$

states are orthogonal $H_{12}^{(0)} = H_{21}^{(0)} = 0$
$H^{(1)}$ is Hermitian $H_{12}^{(1)} = H_{21}^{(1)*}$
$\varepsilon^2 = |H_{12}^{(1)}|^2$

if perturbation is absent, $\varepsilon = 0$ $\quad E_- = E_1^{(0)}$, $\quad E_+ = E_2^{(0)}$



when a perturbation is applied, the lower level moves down in energy and the upper level moves up
the closer the unperturbed states are in energy, the greater the effect of a perturbation
the stronger the perturbation, the greater the effect on the energies of the levels

consider $\varepsilon^2 \ll (E_2^{(0)} - E_1^{(0)})^2$

$$\Rightarrow E_\pm = \frac{1}{2}(E_1^{(0)} + E_2^{(0)}) \pm \frac{1}{2}(E_2^{(0)} - E_1^{(0)})\sqrt{1 + \frac{4\varepsilon^2}{(E_2^{(0)} - E_1^{(0)})^2}}$$

$$= \frac{1}{2}(E_1^{(0)} + E_2^{(0)}) \pm \frac{1}{2}(E_2^{(0)} - E_1^{(0)})\left[1 - \frac{2\varepsilon^2}{\underbrace{(E_2^{(0)} - E_1^{(0)})^2}_{\Delta E^{(0)}}} + \cdots\right]$$

$$\Rightarrow E_- = E_1^{(0)} - \frac{\varepsilon^2}{\Delta E^{(0)}} \qquad E_+ = E_2^{(0)} + \frac{\varepsilon^2}{\Delta E^{(0)}}$$

a convenient way to express the solutions is to write

$$\psi_- = \psi_1^{(0)}\cos\zeta + \psi_2^{(0)}\sin\zeta \qquad \psi_+ = -\psi_1^{(0)}\sin\zeta + \psi_2^{(0)}\cos\zeta \qquad \tan 2\zeta = \frac{2|H_{12}^{(1)}|}{E_2^{(0)} - E_1^{(0)}}$$

Nondegenerate for many level system

$H^{(0)}|n\rangle = E_n^{(0)}|n\rangle \qquad n=0,1,2,\cdots$

suppose we are unable to solve $\hat{H}\psi_n = E_n\psi_n$, assume that $\hat{H}$ is only slightly different from the $\hat{H}^0$ (unperturbed, ≒ ground state)

Ex: $\hat{H} = \underbrace{-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}kx^2}_{\hat{H}^0} + \underbrace{cx^3 + dx^4}_{\hat{H}^1}$ if c and d are small

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

$\psi_0 = \psi_0^{(0)} + \lambda\psi_0^{(1)} + \lambda^2\psi_0^{(2)} + \cdots$

$E_0 = E_0^{(0)} + \lambda \underbrace{E_0^{(1)}}_{\text{first order correction}} + \lambda^2 \underbrace{E_0^{(2)}}_{\text{second order correction}} + \cdots$

$H\psi = E\psi = \lambda^0\left[H^{(0)}\psi_0^{(0)} - E_0^{(0)}\psi_0^{(0)}\right] + \lambda^1\left[H^{(0)}\psi_0^{(1)} + H^{(1)}\psi_0^{(0)} - E_0^{(0)}\psi_0^{(1)} - E_0^{(1)}\psi_0^{(0)}\right] +$
$\lambda^2\left[H^{(0)}\psi_0^{(2)} + H^{(1)}\psi_0^{(1)} + H^{(2)}\psi_0^{(0)} - E_0^{(0)}\psi_0^{(2)} - E_0^{(1)}\psi_0^{(1)} - E_0^{(2)}\psi_0^{(0)}\right] + \cdots = 0$

$\Rightarrow H^{(0)}\psi_0^{(0)} = E_0^{(0)}\psi_0^{(0)}$

$\left[H^{(0)} - E_0^{(0)}\right]\psi_0^{(1)} = \left[E_0^{(1)} - H^{(1)}\right]\psi_0^{(0)}$

$\left[H^{(0)} - E_0^{(0)}\right]\psi_0^{(2)} = \left[E_0^{(2)} - H^{(2)}\right]\psi_0^{(0)} + \left[E_0^{(1)} - H^{(1)}\right]\psi_0^{(1)}$

$\vdots$

the first order correction to the energy

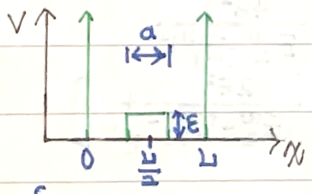
$\psi_0^{(1)} = \sum_n c_n \psi_n^{(0)}$

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

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

$\Rightarrow E_0^{(1)} = \langle 0|H^{(1)}|0\rangle = H_{00}^{(1)}$

Ex:



$a = \frac{L}{10}$

$H^{(1)} = \begin{cases} \varepsilon & \text{if } \frac{1}{2}(L-a) \le x \le \frac{1}{2}(L+a) \\ 0 & \text{otherwise} \end{cases}$

$E_n^{(1)} = \frac{2\varepsilon}{L}\int_{\frac{1}{2}(L-a)}^{\frac{1}{2}(L+a)} \sin^2\left(\frac{n\pi x}{L}\right)dx = \varepsilon\left[\frac{a}{L} - \frac{(-1)^n}{n\pi}\sin\left(\frac{n\pi a}{L}\right)\right]$

$n=1 \quad E^{(1)} = 0.1984\,\varepsilon$
$n=2 \quad E^{(1)} = 0.0065\,\varepsilon$