Teo. de perturbación (t independiente)

Sea $V(x)$ tq. no podemos resolver $\hat{H}|\psi\rangle = E|\psi\rangle$ de manera exacta. Pero $V = V_0 + \Delta V$ donde sabemos como resolver

V_0 → armónico, ΔV → anarmónico

$$\underbrace{\left[\frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V_0(x)\right]}_{H_0} \psi_e^{(0)} = E_e^{(0)} \psi_e^{(0)} \qquad (1)$$

$E_e^{(0)}$, $\psi_e^{(0)}$: conocidos

El sistema "perturbado" obedece: $(H_0 + \Delta V(x))\psi = E\psi$ (2)

Cualq. ψ puede expandirse en términos de los $\{\psi_e^{(0)}\}$:

$$\boxed{\psi_n = \sum_e a_{ne}\psi_e^{(0)}} \qquad (3)$$

$$\Rightarrow (H_0 + \Delta V)\sum_e a_{ne}\psi_e^{(0)} = E_n \sum_e a_{ne}\psi_e^{(0)} \quad / \psi_m^{*(0)} \qquad (3')$$

$$\int \psi_m^{*(0)} (H_0 + \Delta V)\sum_e a_{ne}\psi_e^{(0)} = \int E_n \psi_m^{*(0)} \sum_e a_{ne}\psi_e^{(0)}$$

$$\sum_e a_{ne} \underbrace{\int \psi_m^{*(0)} H_0 \psi_e^{(0)}}_{E_e^{(0)}\delta_{me}} + \sum_e a_{ne} \underbrace{\int \psi_m^{(0)*} \Delta V \psi_e^{(0)} dx}_{\Delta V_{me}} = \sum_e a_{ne} E_n \underbrace{\int \psi_m^{(0)*}\psi_e^{(0)} dx}_{\delta_{em}}$$

$$a_{nm}E_m^{(0)} + \sum_e a_{ne}\Delta V_{me} = a_{nm}E_n$$

$$\therefore \boxed{\sum_e a_{ne}\Delta V_{me} = (E_n - E_m^{(0)})a_{nm}} \qquad (4)$$

Las ecuac. (3) y (4) son exactas.

En el límite $\Delta V_{mn} \to 0$, se espera $a_{nl} \to \delta_{nl}$

$\Rightarrow$ En 1ᵉʳᵃ aprox., ponemos $a_{nl} \simeq \delta_{nl}$

$$\Rightarrow E_n^{(1)} \simeq E_n^{(0)} + (\Delta V)_{nn} = E_n^{(0)} + \int \psi_n^{(0)*} \Delta V \psi_n^{(0)} dx \qquad (5)$$

En 2ᵈᵃ aprox., sup. en (4) que sólo a_{nm} y a_{nn} son $\neq 0$

$$a_{nm} (\Delta V)_{mm} + \underbrace{a_{nn}}_{1} (\Delta V)_{mn} = (E_n^{(1)} - E_m^{(0)}) a_{nm}$$

$$\Rightarrow a_{nm} \left\{ (\Delta V)_{mm} - (E_n^{(1)} - E_m^{(0)}) \right\} = -(\Delta V)_{mn}$$

pero $(\Delta V)_{mm} = E_m^{(1)} - E_m^{(0)}$

$$\Rightarrow \boxed{a_{nm} = \frac{\Delta V_{mn}}{E_n^{(1)} - E_m^{(1)}}} \qquad (n \neq m) \qquad (6)$$

Usando (6), (3) quedaría..

$$\psi_n^{(1)} \simeq \sum_l \frac{(\Delta V)_{ln}}{E_n^{(1)} - E_l^{(1)}} \psi_l^{(0)} \qquad (7)$$

Para un método más sistemático:

$$a_{nl} = \delta_{nl} + a_{nl}^{(1)} + a_{nl}^{(2)} + \cdots$$
$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)}$$

donde la expansión es en órdenes de $|\Delta V|$

$$\Delta V \to \lambda \Delta V \Rightarrow E_n^{(l)} \propto \lambda^l |\Delta V|^l$$

Introduciendo en la ec. EXACTA (4):

$$\sum_l \{\delta_{nl} + a_{nl}^{(1)} + a_{nl}^{(2)} + \cdots\} (\Delta V)_{ml} = (E_n^{(0)} - E_m^{(0)} + E_n^{(1)} + E_n^{(2)} + \cdots)(\delta_{nm} + a_{nm}^{(1)} + \cdots)$$

$$\Rightarrow (\Delta V)_{mn} = (E_n^{(0)} - E_m^{(0)}) a_{nm}^{(1)} + E_n^{(1)} \delta_{nm} \Rightarrow \boxed{a_{nm}^{(1)} = \frac{(\Delta V)_{mn}}{E_n^{(0)} - E_m^{(0)}}} \quad (m \neq n)$$

and $\boxed{E_n^{(1)} = (\Delta V)_{nn}}$

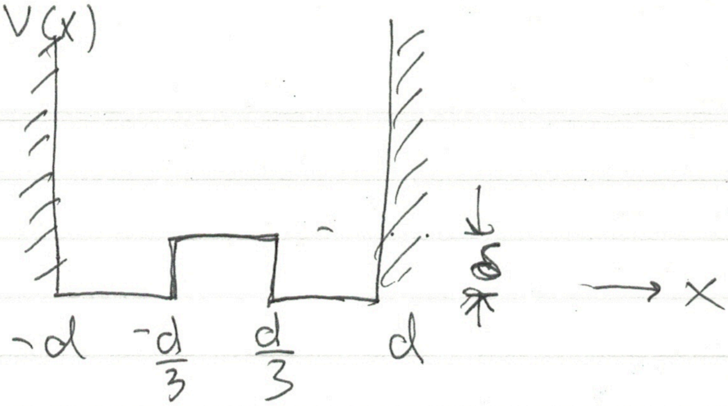
$$\sum_l a_{nl}^{(1)} (\Delta V)_{ml} = E_n^{(2)} \delta_{nm} + E_n^{(1)} a_{nm}^{(1)} + (E_n^{(0)} - E_m^{(0)}) a_{nm}^{(2)}$$

$$n = m \Rightarrow \sum_l a_{nl}^{(1)} (\Delta V)_{nl} = E_n^{(2)} + E_n^{(1)} \underbrace{\cancel{a_{nn}^{(1)}}}_{0}$$

$$E_n^{(2)} = \sum_l \frac{(\Delta V)_{ln}}{E_n^{(0)} - E_l^{(0)}} (\Delta V)_{nl} = \sum_l \frac{(\Delta V)_{nl}^{*} (\Delta V)_{nl}}{E_n^{(0)} - E_l^{(0)}} = \boxed{\sum_{l \neq n} \frac{|\Delta V|_{nl}^2}{E_n^{(0)} - E_l^{(0)}}}$$

$$\Psi_n = \psi_n^{(0)} + \sum_l a_{nl}^{(1)} \psi_l^{(0)} + \sum_l a_{nl}^{(2)} \psi_l^{(0)} + \cdots$$

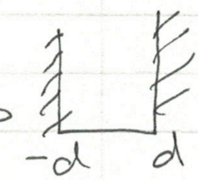
Ejemplo



$$V(x) = \begin{cases} \infty & |x| > d \\ 0 & \frac{d}{3} < |x| < d \\ \delta & |x| < d/3 \end{cases} = V_0(x) + v(x)$$

donde se asume que $\delta \ll \frac{\pi^2 \hbar^2}{8md^2}$

los autofns. "no-perturbados" son los del pozo



$$\psi_n^{(0)} = \begin{cases} N_n \cos\left(\frac{n\pi x}{2d}\right) & n \text{ impar} \\ N_n \sin\left(\frac{n\pi x}{2d}\right) & n \text{ par} \end{cases} \Bigg\} |x| \leq d$$
$$\qquad 0 \qquad |x| \geq d$$

donde $N_d = 1/\sqrt{d}$ $\forall n$.

niveles "no-perturbados" $E_n^{(0)} = \frac{n^2 \hbar^2 \pi^2}{8md^2}$

A 1er orden, $E_n^{(1)} - E_n^{(0)} = \int_{-\infty}^{\infty} \psi_n^{(0)*} v(x) \psi_n^{(0)}(x) dx$

p.ej. $E_1^{(1)} - E_1^{(0)} = \int_{-d/3}^{d/3} \delta\, \psi_1^{(0)*} \psi_1^{(0)} dx = 2\delta \int_0^{d/3} N_1^2 \cos^2\left(\frac{\pi x}{2d}\right) dx$

$$= \frac{2\delta}{d} \cdot \int_0 \cos^2\left(\frac{\pi x}{2d}\right) dx$$

$$= \frac{2\delta}{\cancel{d}} \left(\frac{2\cancel{d}}{\pi}\right) \int_0^{\pi/6} \cos^2(s) ds = \frac{4\delta}{\pi} \cdot \underbrace{\int_0^{\pi/6} \cos^2(x) dx}_{\frac{\pi}{12} + \frac{\sqrt{3}}{8}} = 0.61\delta$$

$$\boxed{E_1 \simeq \frac{\pi^2 \hbar^2}{8md^2} + 0.61\delta}$$

La autofn. perturbada es:

$$\psi_1 = \psi_1^{(0)} + \sum_{l>1} a_{1l} \psi_l^{(0)}$$

a 1er orden,
$$a_{1l} = \frac{\int_{-\infty}^{\infty} \psi_l^{*(0)}(x) V(x) \psi_1^{(0)}(x) dx}{E_1^{(0)} - E_l^{(0)}}$$

Como $V(x)$ es par, y $\psi_1^{(0)}(x)$ es par, $\Rightarrow$ solo l = impar contribuye,

$$a_{13} = \frac{N_1 N_2 \delta \int_{-d/3}^{d/3} \cos\left(\frac{3\pi x}{2d}\right) \cos\left(\frac{\pi x}{2d}\right) dx}{\frac{\pi^2 \hbar^2}{8md^2} (1-9)}$$

$$= \frac{-\delta}{d} \cdot \frac{\cancel{8} m d^2}{\pi^2 \hbar^2 \cancel{8}} \cdot 2 \int_0^{d/3} \cos\left(\frac{3\pi x}{2d}\right) \cos\left(\frac{\pi x}{2d}\right) dx \cdot$$

$$-\frac{2\delta m d}{\pi^2\hbar^2}\int_0^{d/3}\cos\left(\frac{3\pi x}{2d}\right)\cos\left(\frac{\pi x}{2d}\right)dx \qquad s=\frac{\pi x}{2d}, \quad ds=\frac{\pi}{2d}dx$$

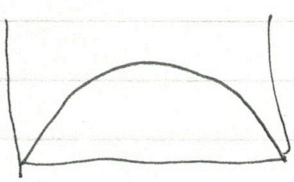
$$=\frac{-2\delta m d}{\pi^2\hbar^2}\cdot\frac{2d}{\pi}\int_0^{\pi/6}\cos(3s)\cos(s)\,ds$$

$$\frac{-4m\delta d^2}{\pi^3\hbar^2}\cdot\underbrace{\int_0^{\pi/6}\cos(3x)\cos(x)\,dx}_{\int_0^{\pi/6}\frac{1}{2}\left[\cos(4x)+\cos(2x)\right]dx}$$

$$\frac{1}{8}\underbrace{\sin\left(\frac{2\pi}{3}\right)}_{\sqrt{3}/2}+\frac{1}{4}\underbrace{\sin\left(\frac{\pi}{3}\right)}_{\sqrt{3}/2}$$

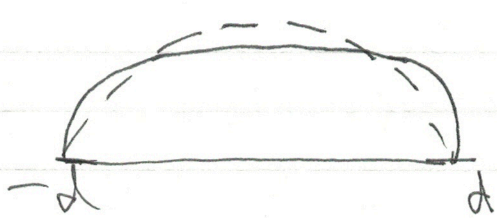
$$=\frac{-4m\delta d^2}{\pi^3\hbar^2}\cdot\frac{3\sqrt{3}}{16}=-\frac{3\sqrt{3}}{4}\frac{md^2\delta}{\pi^3\hbar^2}$$

$$\Rightarrow \boxed{\psi_1\approx\frac{1}{\sqrt{d}}\cos\left(\frac{\pi x}{2d}\right)-\frac{3\sqrt{3}}{4}\frac{md^2\delta}{\pi^3\hbar^2}\cos\left(\frac{3\pi x}{2d}\right)+}$$



+

=



$$a_{1l} = \frac{\int_{-\infty}^{\infty} \psi_l^{(0)*}(x)\, v(x)\, \psi_1^{(0)}(x)\, dx}{E_1^{(0)} - E_l^{(0)}}$$

$v(x) = \text{par}$

$\psi_1^{(0)}(x) = \text{par} \Rightarrow l = \text{impar}$

$$a_{1l} = \frac{N_1 N_l \delta \int_{-d/3}^{d/3} \cos\left(\frac{l\pi x}{2d}\right)\cos\left(\frac{\pi x}{2d}\right) dx}{\frac{\pi^2\hbar^2}{8md^2}(1-\underset{\to\, ??}{9})}$$

$$= \frac{1}{d}\cdot\delta\cdot\frac{8md^2}{(-8)\pi^2\hbar^2}\cdot 2\int_0^{d/3} \cos\left[\frac{l\pi x}{2d}\right]\cos\left[\frac{\pi x}{2d}\right] dx$$

$$= \frac{-2\delta md}{\pi^2\hbar^2}\int_0^{d/3} \cos\left(\frac{l\pi x}{2d}\right)\cos\left(\frac{\pi x}{2d}\right) dx \qquad s = \frac{\pi x}{2d}, \quad dx = \frac{2d}{\pi} ds$$

$$= \frac{-2\delta md}{\pi^2\hbar^2}\cdot\frac{2d}{\pi}\int_0^{\pi/6} \underbrace{\cos(ls)\cos(s)}_{\frac{1}{2}\cos[(l-1)s] + \frac{1}{2}\cos[(l+1)s]} ds$$

$$= \frac{-2m\delta d^2}{\pi^2\hbar^2}\left\{ \underbrace{\int_0^{\pi/6} \cos((l-1)s)\, ds}_{\frac{\sin((l-1)\pi/6)}{l-1}} + \underbrace{\int_0^{\pi/6} \cos((l+1)s)\, ds}_{\frac{\sin[(l+1)\pi/6]}{l+1}} \right\}$$

$$\therefore \quad a_{1l} = \frac{-\delta}{(\pi^2\hbar^2/2md^2)}\left[\frac{\sin[(l-1)\pi/6]}{l-1} + \frac{\sin[(l+1)\pi/6]}{l+1}\right]$$

$$\Psi_1 \approx \frac{1}{\sqrt{d}}\cos\left(\frac{\pi x}{2d}\right) + \left(\frac{-\delta}{\pi^2\hbar^2/2md^2}\right)\sum_{l=3,5,\dots}^{\infty}\left[\frac{\sin((l-1)\pi/6)}{l-1} + \frac{\sin((l+1)\pi/6)}{l+1}\right] \times \cos\left(\frac{l\pi x}{2d}\right)$$

$$+ O\left(\frac{\delta}{\pi^2\hbar^2/2md^2}\right)^2$$

donde $\frac{\delta}{\pi^2\hbar^2/2md^2} \ll 1$ es el parámetro perturbativo.