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

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

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

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

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

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

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

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

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

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

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

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

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

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

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..

$$\psi_n^{(1)} \simeq \sum_\ell \frac{(\Delta V)_{\ell n}}{E_n^{(1)} - E_\ell^{(1)}} \psi_\ell^{(0)} \qquad (7)$$

Para un método más sistemático:

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

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

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

Introduciendo en la ec. <u>EXACTA</u> (4):

$$\sum_\ell \left\{\delta_{n\ell} + a_{n\ell}^{(1)} + a_{n\ell}^{(2)} + \cdots\right\}(\Delta V)_{m\ell} = \left(E_n^{(0)} - E_m^{(0)} + E_n^{(1)} + E_n^{(2)} + \cdots\right)\left(\delta_{nm} + a_{nm}^{(1)} + \cdots\right)$$

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

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

$$\sum_\ell a_{n\ell}^{(1)} (\Delta V)_{m\ell} = E_n^{(2)}\delta_{nm} + E_n^{(1)} a_{nm}^{(1)} + (E_n^{(0)} - E_m^{(0)})\, a_{nm}^{(2)}$$

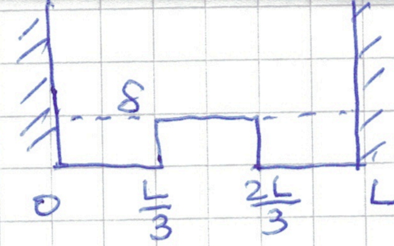
$$n = m \Rightarrow \sum_\ell a_{n\ell}^{(1)} (\Delta V)_{n\ell} = E_n^{(2)} + E_n^{(1)} \cancelto{0}{a_{nn}^{(1)}}$$

$$E_n^{(2)} = \sum_\ell \frac{(\Delta V)_{\ell n}}{E_n^{(0)} - E_\ell^{(0)}} (\Delta V)_{n\ell} = \sum_\ell \frac{(\Delta V)_{n\ell}^{*} (\Delta V)_{n\ell}}{E_n^{(0)} - E_\ell^{(0)}} = \boxed{\sum_{\ell \neq n} \frac{|\Delta V|_{n\ell}^2}{E_n^{(0)} - E_\ell^{(0)}}}$$

$$\psi_n = \psi_n^{(0)} + \sum_\ell a_{n\ell}^{(1)} \psi_\ell^{(0)} + \sum_\ell a_{n\ell}^{(2)} \psi_\ell^{(0)} + \cdots$$

Ejemplo: pozo ∞ con barrera

$\Delta V = \delta$, $\frac{L}{3} < x < \frac{2}{3}L$



$$E_n^{(0)} = \frac{\pi^2 \hbar^2}{2mL^2} n^2 \quad ; \quad \psi_n^{(0)} = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

$$E_n \approx E_n^{(0)} + \int_0^L \psi_n^{0*} \Delta V \psi_n^0 = E_n^0 + \delta \int_{L/3}^{(2/3)L} \sin^2\left(\frac{n\pi x}{L}\right) dx \cdot \left(\frac{2}{L}\right)$$

$$= E_n^{(0)} + \frac{2\delta}{\pi} \int_{\pi/3}^{(2/3)\pi} \sin^2(ns) ds$$

$$= \frac{\pi^2 \hbar^2}{2mL^2} n^2 + \frac{2\delta}{\pi} \left\{ \frac{2n\pi + 3\sin((2/3)\pi n) - 3\sin((4/3)\pi n)}{12n} \right\}.$$

$$n = 1 \Rightarrow \boxed{E_1 \approx \frac{\pi^2 \hbar^2}{2mL^2} + \frac{2}{\pi}\left(\frac{\sqrt{3}}{4} + \frac{\pi}{6}\right)\delta .} \qquad (1)$$

$$\psi_1 \approx \psi_1^{(0)} + \sum_{l>1} a_{1l} \psi_l^{(0)} \qquad (2)$$

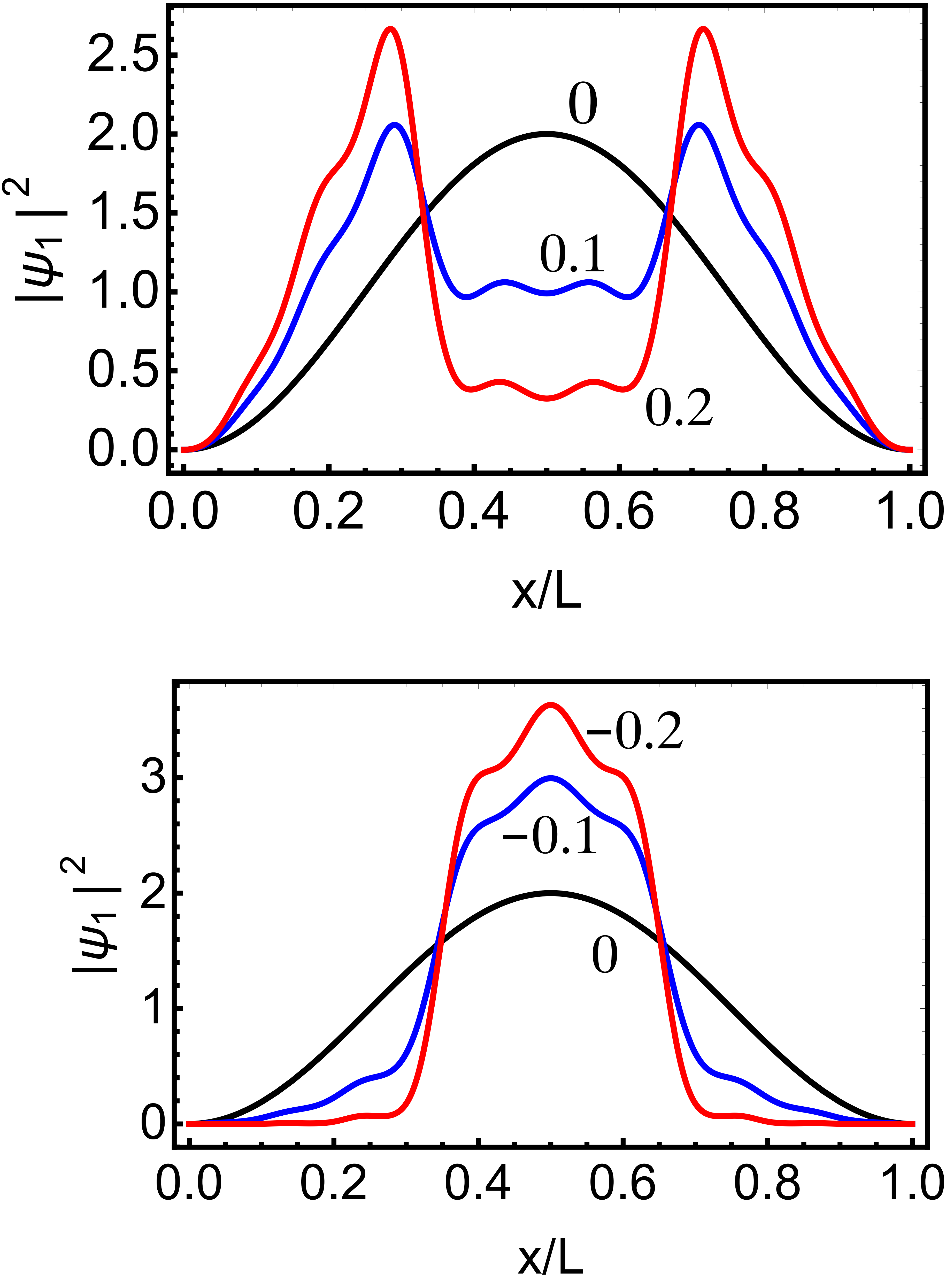
donde, $$a_{1l} = \frac{\int_0^L \psi_1^{(0)*}(x) \Delta V \psi_l^{(0)}(x)}{E_1^{(0)} - E_l^{(0)}} = \frac{(2/L)\delta \int_{L/3}^{(2/3)L} \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{n\pi x}{L}\right)}{\frac{\pi^2\hbar^2}{2mL^2}(1-l^2)}$$

$$= -2\delta \frac{\sin\left(\frac{\ell\pi}{2}\right)\left(\sqrt{3}\,\ell \sin(\ell\pi/6) - \cos(\ell\pi/6)\right)}{\frac{\pi^3\hbar^2}{2mL^2}(1-\ell^2)^2} \qquad (3)$$

∘ sea,

$$\psi_1 \simeq \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right) +$$

$$- \delta \sum_{\ell=2}^{\infty} \frac{2\sqrt{2/L}\,\sin\left(\frac{\ell\pi}{2}\right)\left(\sqrt{3}\,\ell \sin\left(\frac{\ell\pi}{6}\right) - \cos\left(\frac{\ell\pi}{6}\right)\right)\sin\left(\frac{\ell\pi x}{L}\right)}{(\pi^3\hbar^2/2mL^2)(1-\ell^2)^2}.$$



0
0.1
0.2
$|\psi_1|^2$
x/L
-0.2
-0.1
0
$|\psi_1|^2$
x/L

otro ejemplo: perturbación δ

$$V(x) = (L/2)\Omega\,\delta(x-(L/2))$$

calc. E_1 y ψ_1 a 1er orden

$$E_1 \simeq E_1^{(0)} + \int \psi_1^{(0)*} V(x) \psi_1^{(0)}$$

$$= E_1^{(0)} + \cancel{\left(\tfrac{2}{L}\right)}\cancel{\left(\tfrac{L}{2}\right)}\Omega \underbrace{\int_0^L \sin^2\left(\tfrac{\pi x}{L}\right)\delta(x-(L/2))\,dx}_{1}$$

$$\therefore\ E_1 \simeq E_1^{(0)} + \Omega = \frac{\pi^2\hbar^2}{2mL^2} + \Omega .$$

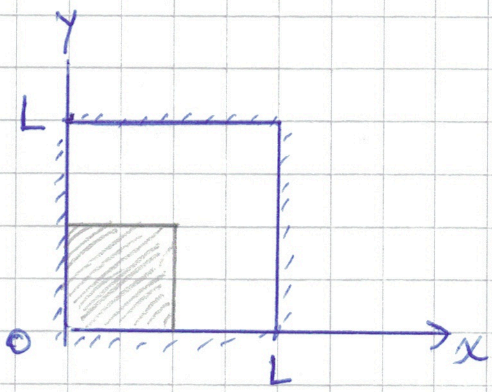
$$\psi_1 \simeq \psi_1^{(0)} + \sum_{l>1} a_{1l}\psi_l^{(0)}$$

$$a_{1l} = \frac{\int_0^L \psi_1^{(0)*} V(x) \psi_l^{(0)}}{E_1^{(0)} - E_l^{(0)}} = \Omega \frac{\int_0^L \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{l\pi x}{L}\right)\delta\left(x-\frac{L}{2}\right)}{\frac{\pi^2\hbar^2}{2mL^2}(1-l^2)}$$

$$= \frac{\Omega}{\pi^2\hbar^2/2mL^2} \cdot \frac{\sin(l\pi/2)}{(1-l^2)}$$

$$\psi_1 \simeq \sqrt{\frac{2}{L}}\sin\left(\frac{\pi x}{L}\right) + \frac{\Omega}{(\pi^2\hbar^2/2mL^2)} \cdot \sum_{l=2}^{\infty} \frac{\sin(l\pi/2)\sin\left(\frac{l\pi x}{L}\right)}{(1-l^2)} .$$

Perturbación en D=2



$$E_{11}^{(0)} = \frac{\pi^2\hbar^2}{2mL^2}(1^2+1^2) = \frac{\pi^2\hbar^2}{mL^2} \qquad (1)$$

$$\psi_{11}^{(0)} = \frac{2}{L}\sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right) \qquad (2)$$

$$V(x,y) = \delta \quad , \quad \begin{array}{l} 0<x<\frac{L}{2} \\ 0<y<L/2 \end{array} \qquad (3)$$

$$E_{11} \simeq E_{11}^{(0)} + \delta\int_0^{L/2}\int_0^{L/2}\left(\frac{4}{L^2}\right)\sin^2\left(\frac{\pi x}{L}\right)\sin^2\left(\frac{\pi y}{L}\right)dx\,dy$$

$$= E_{11}^{(0)} + \frac{\delta}{4} = \frac{\pi^2\hbar^2}{mL^2} + (1/4)\delta \qquad (4)$$

$$\psi_{11} \simeq \psi_{11}^{(0)} + \sum_{l,m\neq 1,1} a_{11,lm}\,\psi_{lm}^{(0)} \quad , \text{ con } a_{11,lm} =$$

$$\text{con } a_{11,lm} = \frac{\iint \psi_{11}^{(0)*}\,V(x,y)\,\psi_{lm}^{(0)}}{E_{11}^{(0)} - E_{lm}^{(0)}} \qquad (5)$$

$$= \frac{\delta \int_0^{L/2}\int_0^{L/2} \left(\frac{4}{L}\right)^2 \sin\left(\frac{\pi x}{L}\right)\sin\left(\frac{\pi y}{L}\right)\sin\left(\frac{\ell \pi x}{L}\right)\sin\left(\frac{\ell \pi y}{L}\right)}{\frac{\pi^2 \hbar^2}{2mL^2}\left(2-\ell^2-m^2\right)}$$

$$= \frac{\left(\frac{4}{\pi}\right)^2 \delta}{\left(\pi^2\hbar^2/2mL^2\right)} \frac{\int_0^{\pi/2}\int_0^{\pi/2} \sin(s)\sin(r)\sin(\ell s)\sin(mr)}{\left(2-\ell^2-m^2\right)}$$

$$= \frac{(4/\pi)^2\,\delta}{\left(\pi^2\hbar^2/2mL^2\right)} \cdot \frac{\ell m \cos(\ell\pi/2)\cos(m\pi/2)}{(2-\ell^2-m^2)(\ell^2-1)(m^2-1)} \qquad (6)$$

Un caso más exótico

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}kx^2$$

$$H = \frac{p^2}{2(m+\Delta m)} + \frac{1}{2}kx^2 \simeq \frac{p^2}{2m} + \frac{1}{2}kx^2 - \frac{\Delta m}{2m^2}p^2$$

$$H = H_0 + \Delta H \,, \quad \Delta H = -\frac{\Delta m}{2m^2}p^2 = +\frac{\Delta m}{2m^2}\hbar^2\frac{\partial^2}{\partial x^2}$$

Conocemos $E_n^{(0)}$ y $\psi_n^{(0)}$.

Calcular E_n a primer orden.

$$a|n\rangle = \sqrt{n}|n-1\rangle$$
$$a^+|n\rangle = \sqrt{n+1}|n+1\rangle$$

$$E_n \simeq -\frac{\Delta m}{2m^2}\langle n|\left(-\frac{\hbar m\omega}{2}\right)(a^+-a)^2|n\rangle$$

$$= \frac{\Delta m}{2m^2}\left(\frac{\hbar m\omega}{2}\right)\underbrace{\langle n|a^{+2}+a^2-a^+a-aa^+|n\rangle}_{-(2n+1)}$$

$$= \frac{-\Delta m}{2m}\left(\frac{\hbar\omega}{2}\right)(2n+1) = -\frac{\Delta m}{2m}\cdot\hbar\omega\left(n+\frac{1}{2}\right).$$

$$\Rightarrow E_n \simeq \hbar\omega\left(n+\frac{1}{2}\right) - \frac{\Delta m}{2m}\hbar\omega\left(n+\frac{1}{2}\right) = \left(1-\frac{\Delta m}{2m}\right)\hbar\omega\left(n+\frac{1}{2}\right) \quad //$$