

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 $\downarrow$ armónico $\nearrow$ anarmónico

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

conocidos

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

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

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

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

$\psi_m^{*(0)}$

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

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

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

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

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

En el límite $\Delta V_{mn} \rightarrow 0$, se espera $Q_{ne} \rightarrow \delta_{ne}$

$\Rightarrow$ En 1^{era} aprox., podemos $Q_{ne} \approx \delta_{ne}$

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

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

$$a_{nm} (\Delta V)_{mn} + \underbrace{a_{nm}}_1 (\Delta V)_{nn} = (E_n^{(1)} - E_m^{(0)}) a_{nm}$$

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

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

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

Usando (6), (3) quedando:

$$\psi_n^{(1)} \approx \sum_e \frac{(\Delta V)_{en}}{E_n^{(1)} - E_e^{(1)}} \psi_e^{(0)} \quad (7)$$

Pour un méthode plus systématique :

$$Q_{ne} = S_{ne} + Q_{ne}^{(1)} + Q_{ne}^{(2)} + \dots$$

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

d'où la expansion en ordres de $|\Delta V|$
 $\Delta V \rightarrow \lambda \Delta V \Rightarrow E_n^{(1)} \propto \lambda^2 |\Delta V|^2$

Introduisant en la ec. EXACTE (4) :

$$\sum_e \{S_{ne} + Q_{ne}^{(1)} + Q_{ne}^{(2)} + \dots\} (\Delta V)_{me} = (E_n^{(0)} - E_m^{(0)} + E_n^{(1)} + E_n^{(2)} + \dots) (S_{nm} + Q_{nm}^{(1)} + \dots)$$

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

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

$$\sum_e Q_{ne}^{(1)} (\Delta V)_{me} = E_n^{(2)} S_{nm} + E_n^{(1)} Q_{nm}^{(1)} + (E_n^{(0)} - E_m^{(0)}) Q_{nm}^{(2)}$$

$$n=m \Rightarrow \sum_e Q_{ne}^{(1)} (\Delta V)_{nn} = E_n^{(2)} + E_n^{(1)} Q_{nn}^{(1)} \rightarrow 0$$

$$E_n^{(2)} = \sum_e \frac{(\Delta V)_{en} (\Delta V)_{ne}}{E_n^{(0)} - E_e^{(0)}} = \sum_e \frac{(\Delta V)_{ne}^* (\Delta V)_{ne}}{E_n^{(0)} - E_e^{(0)}} = \boxed{\sum_{e \neq n} \frac{|\Delta V|_{ne}^2}{E_n^{(0)} - E_e^{(0)}}}$$

$$\Psi_n = \Psi_n^{(0)} + \sum_e Q_{ne}^{(1)} \Psi_e^{(0)} + \sum_e Q_{ne}^{(2)} \Psi_e^{(0)} + \dots$$

Ejemplo: pozo ∞ con barrera

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



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

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

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

$$= \frac{\pi^2 \hbar^2}{2mL^2} n^2 + \frac{2\delta}{\pi} \left\{ \frac{2n\pi + 3\sin((2/3)\pi n) - 3\sin((1/3)\pi n)}{12n} \right\}$$

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

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

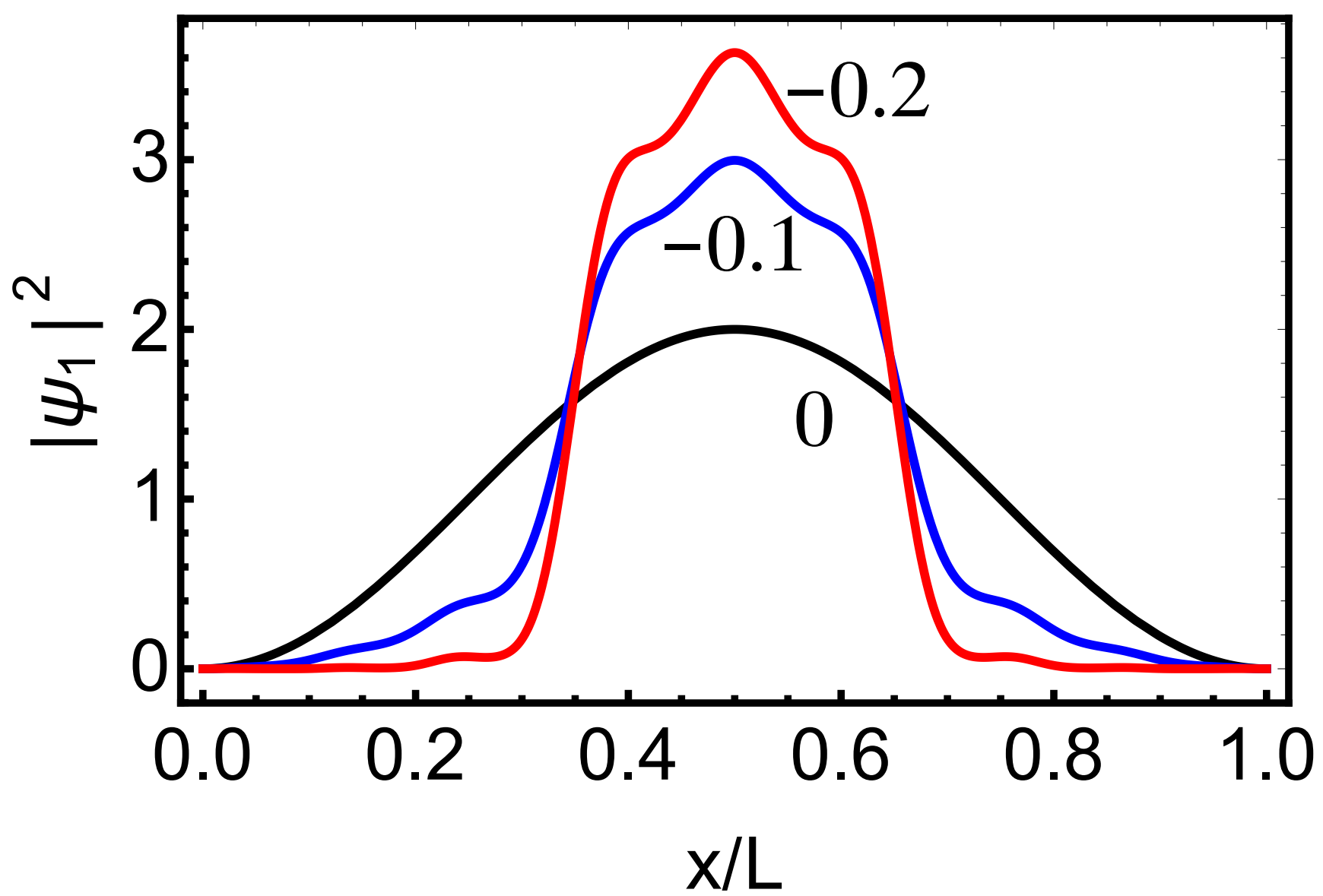
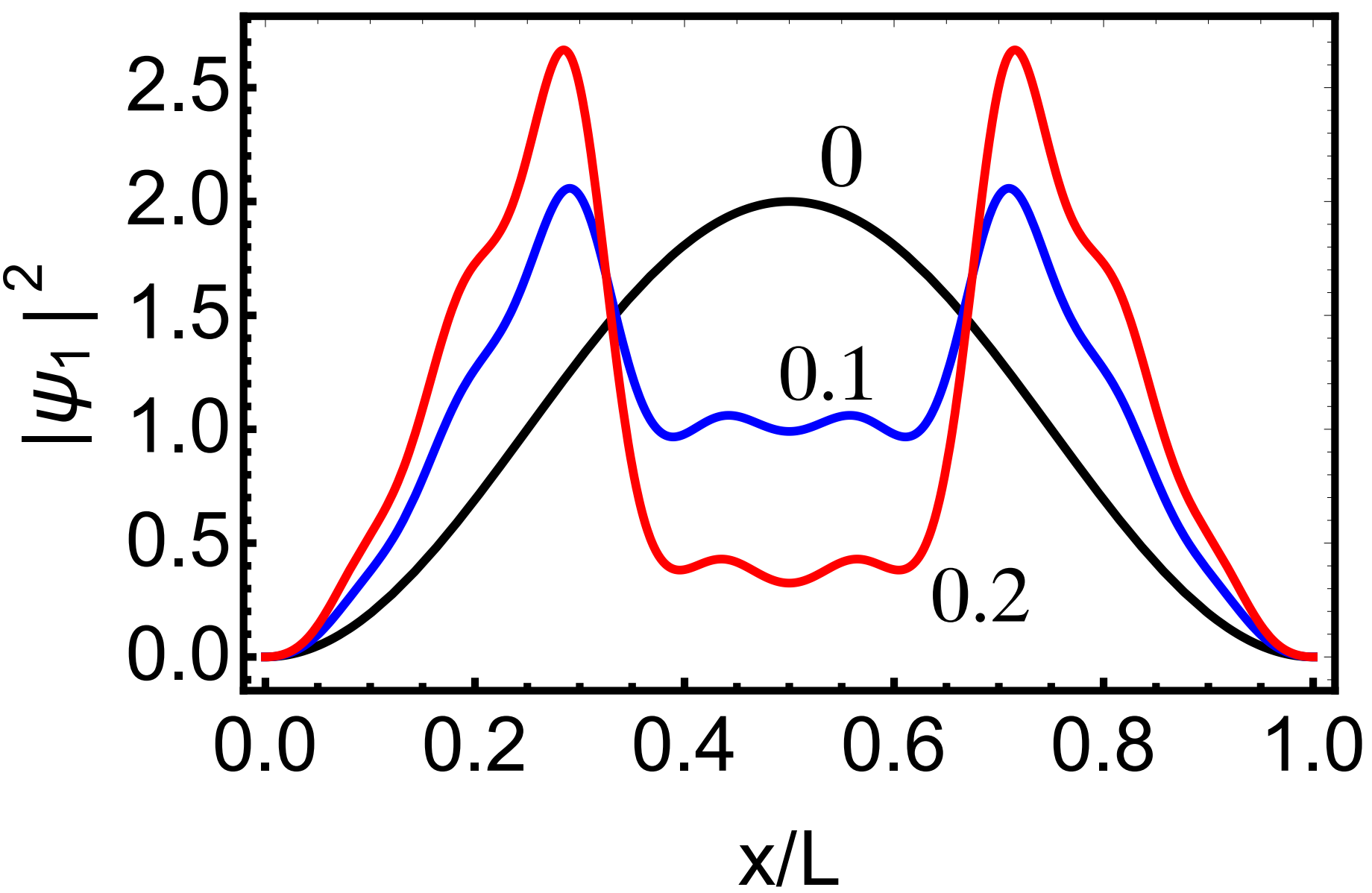
$$\text{donde, } a_{1l} = \frac{\int_0^L \psi_1^{(0)*} \Delta V \psi_l^{(0)} dx}{E_1^{(0)} - E_l^{(0)}} = \frac{(2/L)\delta \int_{L/3}^{(2/3)L} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{l\pi x}{L}\right) dx}{\frac{\pi^2 \hbar^2}{2mL^2} (1-l^2)}$$

$$= -2S \sin\left(\frac{q\pi}{2}\right) \frac{(\sqrt{3}q \sin(q\pi/6) - \cos(q\pi/6))}{\frac{\pi^3 \hbar^2}{2mL^2} (1-q^2)^2} \quad (3)$$

o seq,

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

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



otro ejemplo: perturbación δ



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

calc. E_1 y ψ_1 a 1º orden

$$\begin{aligned} E_1 &\approx E_1^{(0)} + \int \psi_1^{(0)*} V(x) \psi_1^{(0)} dx \\ &= E_1^{(0)} + \cancel{\left(\frac{2}{L}\right)} \cancel{\left(\frac{L}{2}\right)} \Omega \int_0^L \sin^2\left(\frac{\pi x}{L}\right) \delta(x - (L/2)) dx \end{aligned}$$

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

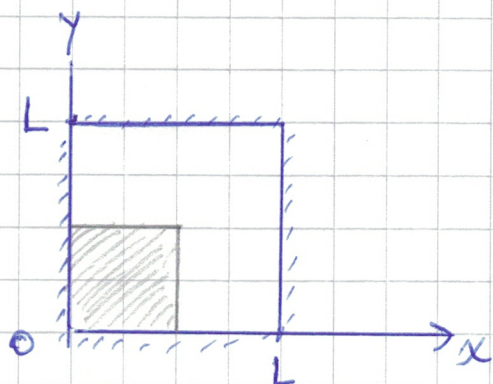
$$\psi_1 \approx \psi_1^{(0)} + \sum_{l>1} a_{1l} \psi_l^{(0)}$$

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

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

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

Perturbación en D=2



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

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

$$V(x,y) = \delta \quad , \quad 0 < x < \frac{L}{2} \\ 0 < y < \frac{L}{2} \quad (3)$$

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

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

$$\psi_{11} \approx \psi_{11}^{(0)} + \sum_{l,m \neq 1,1} a_{11,lm} \psi_{lm}^{(0)}$$

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

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

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

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

un caso más exótico

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

$$H = \frac{p^2}{2(m+\Delta m)} + \frac{1}{2} k x^2 \approx \frac{p^2}{2m} + \frac{1}{2} k x^2 - \frac{\Delta m}{2m^2} p^2$$

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

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

Calcular E_n a primer orden.

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

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

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

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

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