Teoría de Perturbaciones

Ejemplos del caso no degenerado

$H = H_0 + W$ $\qquad |\varphi_n^i\rangle$ e-vectores de H_0

$\qquad\qquad\qquad E_n^0$ e-valores de H_0

Correcciones a primer orden

$$\boxed{\begin{aligned} |\psi_n(\lambda)\rangle &= |\varphi_n\rangle + \lambda \sum_{p\neq n}\sum_i \frac{\langle\varphi_p^i|\hat{W}|\varphi_n\rangle}{E_n^0 - E_p^0}|\varphi_p^i\rangle \\ E_n(\lambda) &= E_n^0 + \lambda\langle\varphi_n|\hat{W}|\varphi_n\rangle \end{aligned}}$$

$$\boxed{\begin{aligned} E(\lambda) &= E_n^0 + \lambda\langle\varphi_n|\hat{W}|\varphi_n\rangle + \lambda^2\sum_{p\neq n}\sum_i \frac{|\langle\varphi_p^i|\hat{W}|\varphi_n\rangle|^2}{E_n^0 - E_p^0} \\ &= \underbrace{E_n^0}_{\text{orden } 0} + \underbrace{\langle\varphi_n|W|\varphi_n\rangle}_{\text{orden } 1} + \underbrace{\sum_{p\neq n}\sum_i \frac{|\langle\varphi_p^i|W|\varphi_n\rangle|^2}{E_n^0 - E_p^0}}_{\text{orden } 2} \end{aligned}}$$

Ejemplo 1: Sistema de 2 niveles

$$H_0 = \begin{pmatrix} E_1 & 0 \\ 0 & E_2 \end{pmatrix} \qquad \text{base } |1\rangle, |2\rangle$$

$$\hat{W}_1 = \begin{pmatrix} \Delta & 0 \\ 0 & \Delta \end{pmatrix} \qquad \hat{W}_2 = \begin{pmatrix} 0 & \Omega \\ \Omega & 0 \end{pmatrix} \quad \text{(tarea)}$$

Ejemplo 2: Oscilador armónico cargado en un campo eléctrico

$$H(\mathcal{E}) = \underbrace{\frac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2}_{H_0} \underbrace{- q\mathcal{E}X}_{W}$$

llamaremos $|\varphi_n\rangle$ los e-vectores de H_0

Solución analítica

$$H|\psi\rangle = E|\psi\rangle$$

en la base $\{|x\rangle\}$ $\langle x|H|\psi\rangle = E\langle x|\psi\rangle$

con $H(\mathcal{E}) = \dfrac{P^2}{2m} + \frac{1}{2}m\omega^2 X^2 - q\mathcal{E}X$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2x^2 - q\mathcal{E}x\right]\psi(x) = E\,\psi(x)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2\left(x^2 - 2\frac{q\mathcal{E}}{m\omega^2}x\right)\right]\psi(x) = E\,\psi(x)$$

Completando cuadrado

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2\left(x - \frac{q\mathcal{E}}{m\omega^2}\right)^2 - \underbrace{\frac{q^2\mathcal{E}^2}{m^2\omega^4}\frac{1}{2}m\omega^2}_{-\frac{q^2\mathcal{E}^2}{2m\omega^2}}\right]\psi(x) = E\psi(x)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + \frac{1}{2}m\omega^2\left(x - \frac{q\mathcal{E}}{m\omega^2}\right)^2\right]\psi(x) = \left[E + \frac{q^2\mathcal{E}^2}{2m\omega^2}\right]\psi(x)$$

Haciendo cambio de variable $x - \dfrac{q\mathcal{E}}{m\omega^2} \to u$

$\dfrac{d}{dx} \to \dfrac{d}{du}$;

$$\tilde{\psi}(u) = \psi(x) = \psi\left(u + \frac{q\mathcal{E}}{m\omega^2}\right)$$

$$\tilde{\psi}(u) = \tilde{\psi}\left(x - \frac{q\mathcal{E}}{m\omega^2}\right)$$

$$\left[-\frac{\hbar^2}{2m}\frac{d^2}{du^2} + \frac{1}{2}m\omega^2u^2\right]\tilde{\psi}(u) = \underbrace{\tilde{E}}_{E + \frac{q^2\mathcal{E}^2}{2m\omega^2}}\,\tilde{\psi}(u)$$

Ecuación del oscilador armónico cuántico

$$\tilde{E}_n = \hbar\omega\left(n+\tfrac{1}{2}\right) \Rightarrow E_n = \tilde{E}_n - \frac{q^2\mathcal{E}^2}{2m\omega^2} = \hbar\omega\left(n+\tfrac{1}{2}\right) - \frac{q^2\mathcal{E}^2}{2m\omega^2}$$

$$\tilde{\psi}_n(u) = \varphi_n(u)$$

$$\psi_n(x) = \varphi_n\left(x - \frac{q\mathcal{E}}{m\omega^2}\right)$$

∴ Las soluciones obtenidas son las del oscilador armónico simple con un corrimiento en energía $-\frac{q^2\mathcal{E}^2}{2m\omega^2}$ y desplazadas en posición por $-\frac{q\mathcal{E}}{m\omega^2}$ pero conservando su forma.

Para poder comparar con el resultado dado por teoría de perturbaciones debemos de escribir $\varphi_n\left(x-\frac{q\mathcal{E}}{m\omega^2}\right)$ en términos de $\varphi_n(x)$.

$$\psi_n(x) = \varphi_n\left(x - \frac{q\mathcal{E}}{m\omega^2}\right)$$

Para que la perturbación sea pequeña $\frac{q\mathcal{E}}{m\omega^2} \ll \sqrt{\frac{\hbar}{m\omega}}$

$$\psi_n(x) = \varphi_n\Big(x - \underbrace{\frac{q\mathcal{E}}{m\omega^2}}_{\Delta x}\Big)$$

$$= \varphi_n(x) - \varphi_n'(x)\frac{q\mathcal{E}}{m\omega^2} + \frac{\varphi_n''(x)}{2!}\left(\frac{q\mathcal{E}}{m\omega^2}\right)^2 + \cdots$$

$$= \left(1 - \frac{q\mathcal{E}}{m\omega^2}\frac{d}{dx} + \left(\frac{q\mathcal{E}}{m\omega^2}\right)^2\frac{d^2}{dx^2} + \cdots\right)\varphi_n(x)$$

$$= \left[\sum_{s=0}^{\infty}\frac{1}{s!}\left(-\frac{q\mathcal{E}}{m\omega^2}\frac{d}{dx}\right)^s\right]\varphi_n(x)$$

$$= e^{-\frac{q\mathcal{E}}{m\omega^2}\frac{d}{dx}}\varphi_n(x) \underset{P=-i\hbar\frac{d}{dx}}{=} e^{-i\frac{q\mathcal{E}}{\hbar m\omega^2}P}\varphi_n(x)$$

en general

$$\underbrace{|\psi_n\rangle}_{\text{e-vector de } H \text{ con perturbación}} = e^{-i\frac{q\mathcal{E}}{\hbar m\omega^2}P}\underbrace{|\varphi_n\rangle}_{\text{e-vector de } H_0} = e^{-\frac{\lambda}{\sqrt{2}}(a^\dagger - a)}|\varphi_n\rangle$$

$$P = i\sqrt{\frac{m\hbar\omega}{2}}(a^\dagger - a)$$

$$\lambda = -\frac{q\mathcal{E}}{\hbar\omega}\sqrt{\frac{\hbar}{m\omega}}$$

$$|\psi_n\rangle = e^{-\frac{\lambda}{\sqrt{2}}(a^+-a)}|\varphi_n\rangle \approx \left[1-\frac{\lambda}{\sqrt{2}}(a^+-a)+\cdots\right]|\varphi_n\rangle$$

$$= |\varphi_n\rangle - \lambda\sqrt{\frac{n+1}{2}}\,|\varphi_{n+1}\rangle + \lambda\sqrt{\frac{n}{2}}\,|\varphi_{n-1}\rangle + \cdots$$

$a^+|\varphi_n\rangle = \sqrt{n+1}\,|\varphi_{n+1}\rangle \qquad a|\varphi_n\rangle = \sqrt{n}\,|\varphi_{n-1}\rangle$

Usando teoría de perturbaciones

$$H(\mathcal{E}) = \underbrace{\frac{P^2}{2m}+\frac{1}{2}m\omega^2X^2}_{H_0}\;\underbrace{-\,q\mathcal{E}X}_{W}$$

$$W = -q\mathcal{E}X = -q\mathcal{E}\sqrt{\frac{\hbar}{m\omega}}\,\hat{X} = \lambda\hbar\omega\hat{X} = \frac{\lambda\hbar\omega}{\sqrt{2}}(a^++a)$$

Con e-vectores $|\varphi_n\rangle$ y e-valores $E_n^0 = \hbar\omega(n+\frac{1}{2})$

¿Cómo cambia la energía de estado n a primer orden en T.P.?

$$E_n = E_n^0 + \langle\varphi_n|W|\varphi_n\rangle = \hbar\omega(n+\tfrac{1}{2}) + \overbrace{\frac{\lambda\hbar\omega}{\sqrt{2}}\langle\varphi_n|a^++a|\varphi_n\rangle}$$

$$= \hbar\omega\,(n+\tfrac{1}{2})$$

No hay corrección a primer orden.
Es necesario calcular 2° orden para obtener una corrección

$$E_n = E_n^0 + \cancel{\langle\varphi_n|W|\varphi_n\rangle}^{\,0} + \sum_{m\neq n}\frac{|\langle\varphi_m|W|\varphi_n\rangle|^2}{E_n^0-E_m^0}$$

$$\langle\varphi_m|W|\varphi_n\rangle = \frac{\lambda\hbar\omega}{\sqrt{2}}\langle\varphi_m|a^++a|\varphi_n\rangle$$

$$= \frac{\lambda\hbar\omega}{\sqrt{2}}\left[\sqrt{n+1}\,\langle\varphi_m|\varphi_{n+1}\rangle + \sqrt{n}\,\langle\varphi_m|\varphi_{n-1}\rangle\right]$$

$$E_n^0-E_m^0 = \hbar\omega(n+\tfrac{1}{2}-m-\tfrac{1}{2}) = \hbar\omega(n-m)$$

$$= \frac{\lambda\hbar\omega}{\sqrt{2}}\left[\sqrt{n+1}\,\delta_{m,n+1} + \sqrt{n}\,\delta_{m,n-1}\right]$$

A segundo orden

$$E_n = \hbar\omega(n+\tfrac{1}{2}) - \underbrace{\frac{\lambda^2\hbar^2\omega^2}{2}\frac{(n+1)}{\hbar\omega}}_{m=n+1} + \underbrace{\frac{\lambda^2\hbar^2\omega^2}{2}\frac{n}{\hbar\omega}}_{m=n-1}$$

$$= \hbar\omega\left[(n+\tfrac{1}{2}) - \frac{\lambda^2}{2}(\cancel{n}+1) + \cancel{\frac{\lambda^2}{2}n}\right]$$

$$= \hbar\omega\left[(n+\tfrac{1}{2}) - \frac{\lambda^2}{2}\right] = \hbar\omega(n+\tfrac{1}{2}) - \frac{q^2\mathcal{E}^2}{2m\omega^2}$$

El resultado analítico es

$$E_n = \hbar\omega(n+\tfrac{1}{2}) - \frac{q^2\mathcal{E}^2}{2m\omega^2}$$ (son idénticos).

¿Como cambia el eigenvector n a primer orden?

$$|\psi_n(\lambda)\rangle = |\varphi_n\rangle + \sum_{m\neq n}\frac{\langle\varphi_m|W|\varphi_n\rangle}{E_n^0 - E_m^0}|\varphi_m\rangle$$

$$\langle\varphi_m|W|\varphi_n\rangle = \frac{\lambda\hbar\omega}{\sqrt{2}}\left[\sqrt{n+1}\,\delta_{m,n+1} + \sqrt{n}\,\delta_{m,n-1}\right]$$

$$|\psi_n\rangle = |\varphi_n\rangle - \frac{\lambda\hbar\omega}{\sqrt{2}}\frac{\sqrt{n+1}}{\hbar\omega}|\varphi_{n+1}\rangle + \frac{\lambda\hbar\omega}{\sqrt{2}}\frac{\sqrt{n}}{\hbar\omega}|\varphi_{n-1}\rangle$$

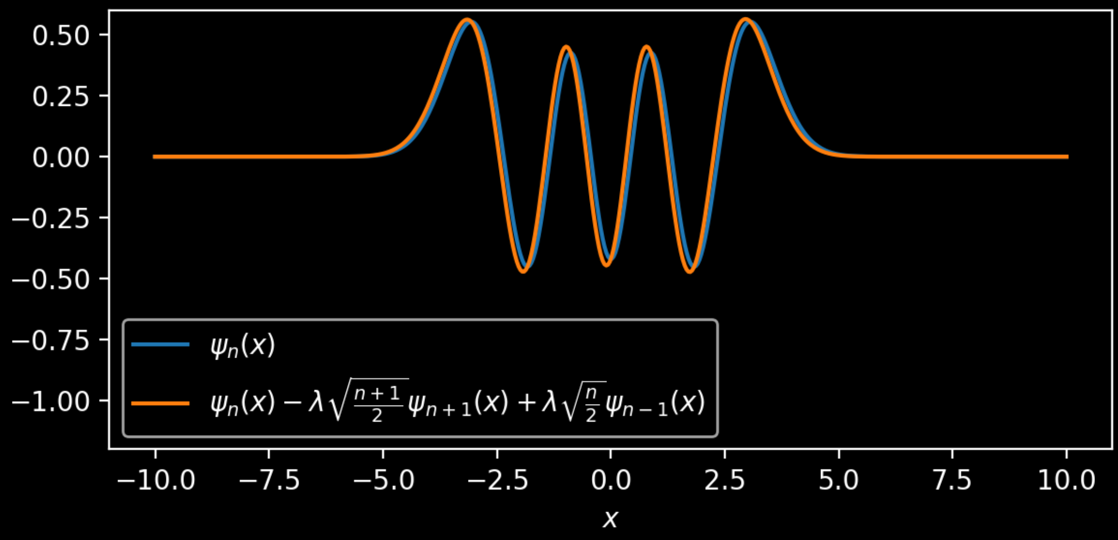
$m=n+1$

$$= |\varphi_n\rangle - \lambda\sqrt{\frac{n+1}{2}}|\varphi_{n+1}\rangle + \lambda\sqrt{\frac{n}{2}}|\varphi_{n-1}\rangle$$

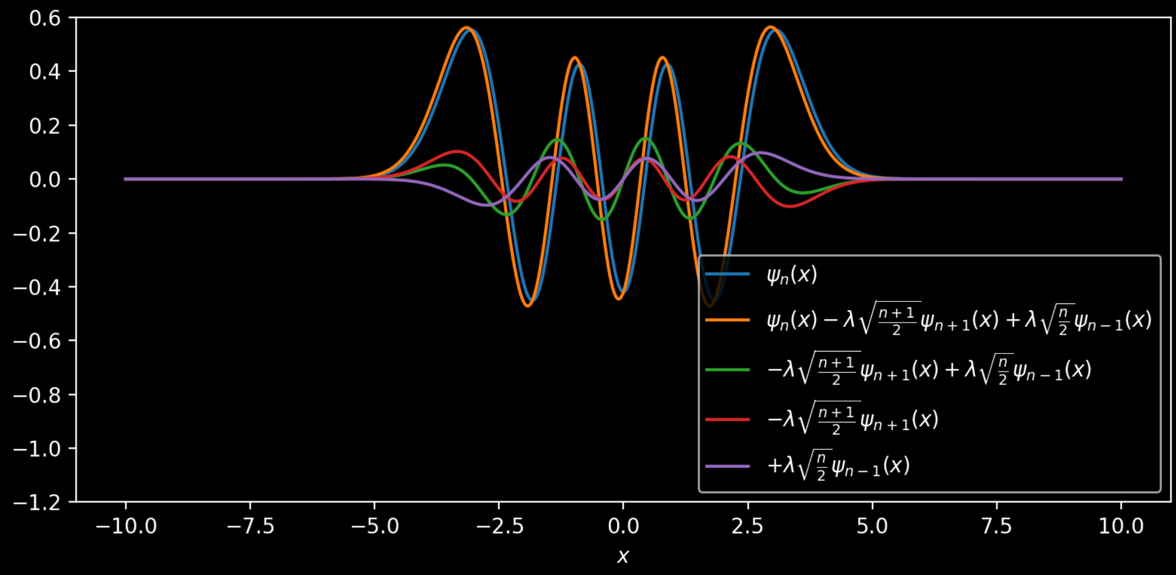
El resultado analítico es

$$|\psi_n\rangle = |\varphi_n\rangle - \lambda\sqrt{\frac{n+1}{2}}|\varphi_{n+1}\rangle + \lambda\sqrt{\frac{n}{2}}|\varphi_{n-1}\rangle + \dots$$

Ojo: el e-vector no es idéntico en ambos casos pues el analítico tiene "..."



$\psi_n(x)$
$\psi_n(x) - \lambda\sqrt{\frac{n+1}{2}}\psi_{n+1}(x) + \lambda\sqrt{\frac{n}{2}}\psi_{n-1}(x)$
x



$\psi_n(x)$
$\psi_n(x) - \lambda\sqrt{\frac{n+1}{2}}\psi_{n+1}(x) + \lambda\sqrt{\frac{n}{2}}\psi_{n-1}(x)$
$-\lambda\sqrt{\frac{n+1}{2}}\psi_{n+1}(x) + \lambda\sqrt{\frac{n}{2}}\psi_{n-1}(x)$
$-\lambda\sqrt{\frac{n+1}{2}}\psi_{n+1}(x)$
$+\lambda\sqrt{\frac{n}{2}}\psi_{n-1}(x)$
x