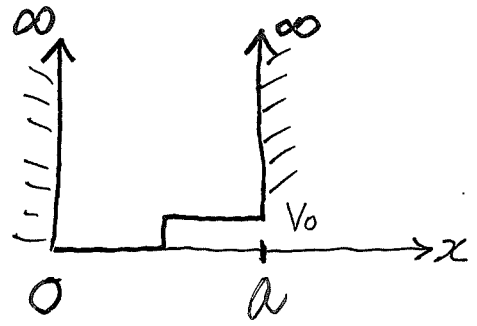
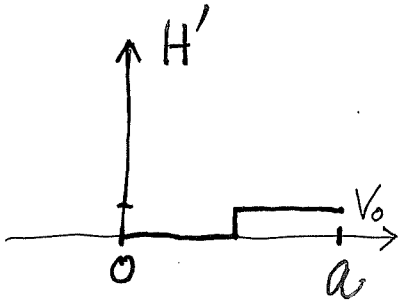
D. Example

A step in 1D infinite well





Unperturbed system: $E_n^{(0)} = \frac{n^2\pi^2\hbar^2}{2ma^2}$; $\psi_n^{(0)} = \sqrt{\frac{2}{a}}\sin\left(\frac{n\pi x}{a}\right)$, $n=1,2,3,\cdots$

Q: Shift in energy for ground state by perturbation theory?

[1st order] $E_1^{(1)}$ ← 1st order shift; G.S. ↗

$$= \int_0^a \psi_1^{*(0)}\hat{H}'\psi_1^{(0)}\,dx = \frac{2}{a}\int_{a/2}^a V_0\sin^2\left(\frac{\pi x}{a}\right)dx = \frac{V_0}{2} \quad \text{(Ex.)}$$

[2nd order] Need $\int_0^L \psi_m^{*(0)}\hat{H}'\psi_1^{(0)}\,dx = \frac{2}{a}V_0\int_{a/2}^a \sin\left(\frac{m\pi x}{a}\right)\cdot\sin\left(\frac{\pi x}{a}\right)dx$ ($m\neq 1$)

$$= \frac{2V_0}{\pi}\int_{\pi/2}^{\pi}\sin(my)\sin y\,dy = \frac{2V_0}{\pi}\,\frac{m\cos\left(\frac{m\pi}{2}\right)}{m^2-1} \quad \text{(Ex.)}$$

$$= \begin{cases} \frac{2V_0}{\pi}\,\frac{m\cos\left(\frac{m\pi}{2}\right)}{m^2-1} & \text{for } m=2,4,6,\cdots \\ 0 & \text{for } m=3,5,7,\cdots \quad [\text{Why so?}] \end{cases}$$

$$\therefore E_1 \approx E_1^{(0)} + E_1^{(1)} + E_1^{(2)} \approx \frac{\pi^2\hbar^2}{2ma^2} + \frac{V_0}{2} + \sum_{m=2,4,\cdots} \frac{4V_0^2}{\pi^2} \frac{m^2\cos^2\left(\frac{m\pi}{2}\right)}{(m^2-1)^2} \frac{1}{\left(\frac{\pi^2\hbar^2}{2ma^2}\right)(1-m^2)}$$

0^{th} order; 1^{st} order (shift up)

- 2^{nd} order [pushed down by $m=2,4,\cdots$ states]
- Most important term is $m=2$, effect drops as m increases

By-product:

$$\psi_1 \approx \psi_1^{(0)} + \psi_1^{(1)} \approx \psi_1^{(0)} + \sum_{m=2,4,\cdots} \frac{2V_0}{\pi} \frac{m\cos\left(\frac{m\pi}{2}\right)}{m^2-1} \cdot \frac{1}{\left(\frac{\pi^2\hbar^2}{2ma^2}\right)(1-m^2)} \cdot \psi_m^{(0)}$$

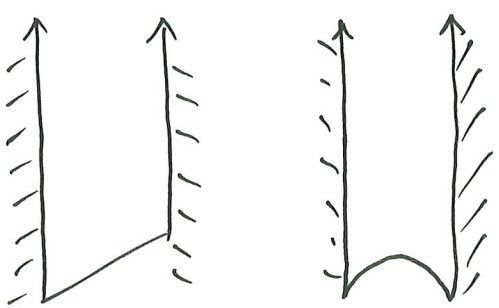
up to 1^{st} order

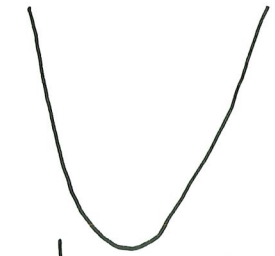
- mix in $\psi_2^{(0)}, \psi_4^{(0)}, \cdots$ to $\psi_1^{(0)}$
- most important mixing from $\psi_2^{(0)}$, other drops as m increases

Extensions

- Relate results here to variational approach using $\phi_{trial} = c_1\psi_1^{(0)} + c_2\psi_2^{(0)}$
- Think: What perturbation theory tells us what variational method doesn't?

Try

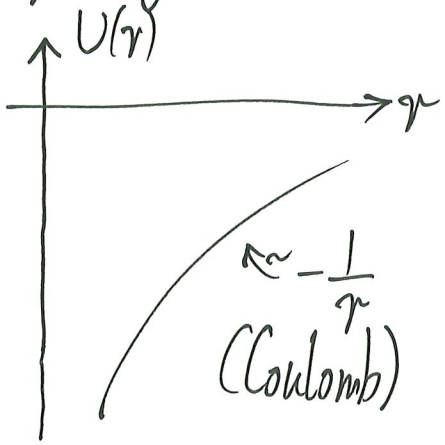




anharmonic oscillator

oscillator with quartic term

Hydrogen Atom + (something)



$+$ { electric field (atomic polarizability)
magnetic field (Zeeman effects)
spin-orbit coupling (total angular momentum)
relativistic correction
$\vdots$

Helium Atom

$$\hat{H}_{\text{Helium}} = \left(\frac{-\hbar^2}{2m}\nabla_{\vec{r}_1}^2 - \frac{2e^2}{4\pi\varepsilon_0 r_1}\right) + \left(\frac{-\hbar^2}{2m}\nabla_{\vec{r}_2}^2 - \frac{2e^2}{4\pi\varepsilon_0 r_2}\right) + \overbrace{\frac{e^2}{4\pi\varepsilon_0|\vec{r}_1 - \vec{r}_2|}}^{\hat{H}'}$$

(a real problem)