Time Independent Perturbation Theory

T.I. S.E. (1-d, p.25, 2.5)
(3-d, p.132, 4.8)

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2} \text{ or } \nabla^2\right)\psi + V\left(\begin{smallmatrix} x \text{ or} \\ \vec{r} \end{smallmatrix}\right)\psi = E\psi$$

Usually, can only solve exactly for an idealized Hamiltonian.

For example

- $-\frac{\hbar^2}{2m}\nabla^2 \leftrightarrow \frac{\hat{p}^2}{2m}$ non-relativistic!

relativistic kinetic energy is... $\sqrt{(mc^2)^2+(cp)^2} - mc^2$

$$(mc^2)\sqrt{1+\frac{p^2}{m^2c^2}} - mc^2$$

$$mc^2\left(1+\frac{p^2}{2m^2c^2}+\frac{1}{2}\left(\frac{1}{2}\right)\left(-\frac{1}{2}\right)\frac{p^4}{m^4c^4}\right) - mc^2$$

$$= \frac{p^2}{2m} - \frac{p^4}{8m^3c^2} \Leftrightarrow \frac{\hat{p}^2}{2m} - \frac{\hat{p}^2}{8m}\left(\frac{\hat{p}^2}{m^2c^2}\right)$$

small in NR problems

- Hydrogen atom... proton not a point charge.. spherical "smear", $r \sim 10^{-13}$ cm

Tiny addition (like $\frac{\hat{p}^4}{8m^3c^2}$) called a <u>perturbation</u>.

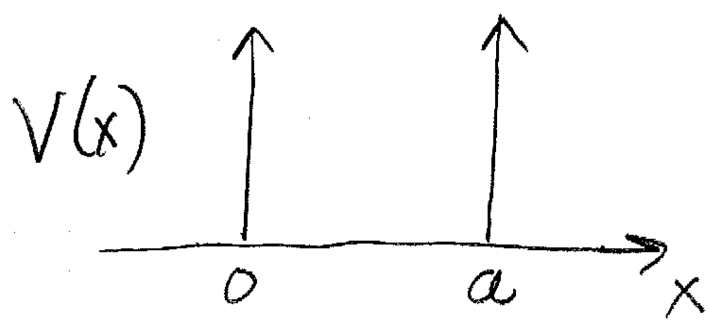
<u>Idea</u>: Suppose we've solved the <u>idealized</u> problem:

Idealized Hamiltonian:

$$H^0 \to \frac{\hat{p}^2}{2m} + V(\hat{x})$$

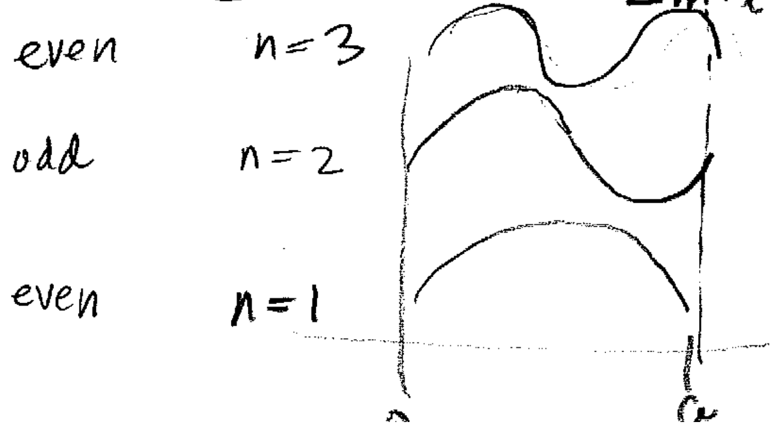
$$\underline{\underline{H^0 \psi_n^0 = E_n^0 \psi_n^0}}$$

<u>Simplest example</u>:



$$n=1,2,3,\dots \quad \begin{cases} \psi_n^0(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \\ E_n^0 = \frac{n^2 \pi^2 \hbar^2}{2ma^2} \end{cases}$$

p. 32



n = # antinodes

n+1 = # nodes

Next Simplest

$$V(x) = \frac{1}{2}kx^2 \qquad \text{S.H.O}$$

Change of variable: $\xi = \sqrt{\frac{m\omega}{\hbar}}\, x$

$$\psi_n^0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{1/4} \frac{1}{\sqrt{2^n n!}} H_n(\xi)\, e^{-\xi^2/2}$$

$$E_n^0 = \left(n+\frac{1}{2}\right)\hbar\omega \qquad n = 0, 1, 2, \ldots$$

$$\omega = \sqrt{\frac{k}{m}} \qquad \text{pp. } 54-56$$

Orthonormality:

$$\underbrace{\int_{0,-\infty}^{a,\infty} dx\, \psi_n^0(x)\, \psi_m(x)}_{} = \delta_{nm}$$

more generally $\quad \underbrace{\langle \psi_n^0 | \psi_m^0 \rangle}_{} = \delta_{nm}$

includes possibility of momentum space, for example

What if $H \neq H^0$, but is CLOSE?

Does knowing E_n^0, ψ_n^0 HELP?

Recall... $\{\psi_n^0\}$ do form a <u>complete set</u>...

$\boxed{\text{Step \#1}}$: <u>accounting</u> $H = H^0 + \lambda H'$

λ is an accounting device, an is DIMENSIONLESS, and, $\lambda \ll 1$

$\lambda \to 0$, $H = H^0$

(In reality... $\langle H' \rangle \ll \langle H^0 \rangle$ too).

$$H \psi_n = E_n \psi_n$$

not H^0 NOT ψ_n^0 not E_n^0

<u>Ansatz</u>:

$$E_n = E_n^0 + \lambda \underbrace{(\#)} + \lambda^2 \underbrace{\binom{\text{other}}{\#}} + \ldots$$

COMPUTE

$$= E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \ldots$$

superscripts <u>not</u> raising to power!

$$\psi_n = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \ldots$$

$\psi_n^1 \to$ a whole function

ψ_n^2 etc.

OBJECTIVE: Find the E_n^i, ψ_n^i

Just Plug in & collect terms of similar power

$$(H^0 + \lambda H')(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \ldots\ldots)$$

$$= (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \ldots)(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 \ldots$$

$\boxed{\text{Step\#2}}$ collect terms of same power in λ

λ^0: $\quad H^0 \psi_n \qquad E_n^0 \psi_n^0$

λ^1 $\quad + \lambda H^0 \psi_n^1 + \lambda H' \psi_n^0 \qquad \lambda E_n^0 \psi_n^1 + \lambda E_n^1 \psi_n^0$

$+\lambda^2 H^0 \psi_n^2 + \lambda^2 H' \psi_n^1 \qquad \lambda^2 E_n^0 \psi_n^2 + \lambda^2 E_n^1 \psi_n^1 + \lambda^2 E_n^2 \psi_n^0$

etc $\quad = \quad$ etc.

Concept: look at terms in a given order in λ, set them individually equal

$\lambda^0 \to$ obviously OK

Step #3 $H^0\psi_n^1 + H^1\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0$

"Project on to ψ_n^0"

$$\langle\psi_n^0|H^0\psi_n^1\rangle + \langle\psi_n^0|H^1\psi_n^0\rangle = \langle\psi_n^0|E_n^0\psi_n^1\rangle + \langle\psi_n^0|E_n^1\psi_n^0\rangle$$

Hermitian

$$E_n^0\cancel{\langle\psi_n^0|\psi_n^1\rangle} + \langle\psi_n^0|H'|\psi_n^0\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle + E_n^1\langle\psi_n^0|\psi_n^0\rangle$$

1

$$\boxed{E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle}$$

meaning...

if $H = H^0 + \cancel{\lambda}^{1} H'$

$$E_n \simeq E_n^0 + \cancel{\lambda}^{1}\langle\psi_n^0|H'|\psi_n^0\rangle + O(\cancel{\lambda^2})$$

h.o.

Sleight of hand... set $\lambda = 1$!

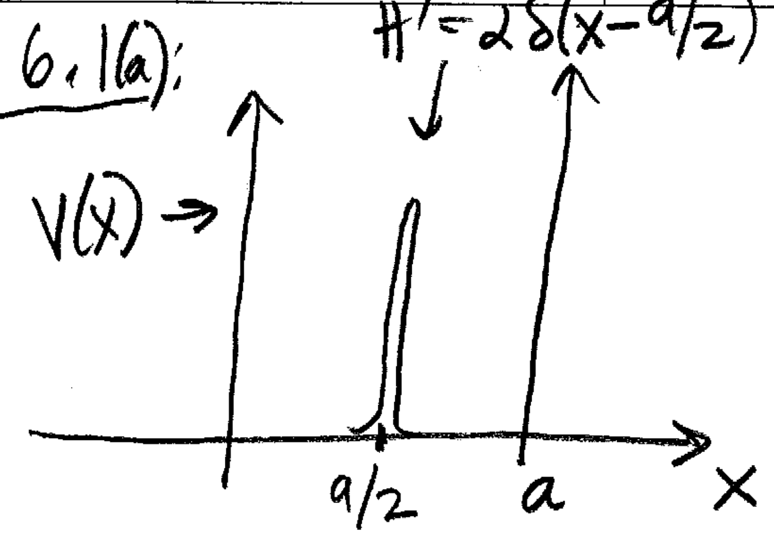
Series only converges if...

further terms involving

H' decrease..

ASSUME THAT

Problem 6.1(a):



$$H^0 = \frac{\hat{p}^2}{2m} + V(x) \qquad H' = \alpha\delta(x - a/2)$$

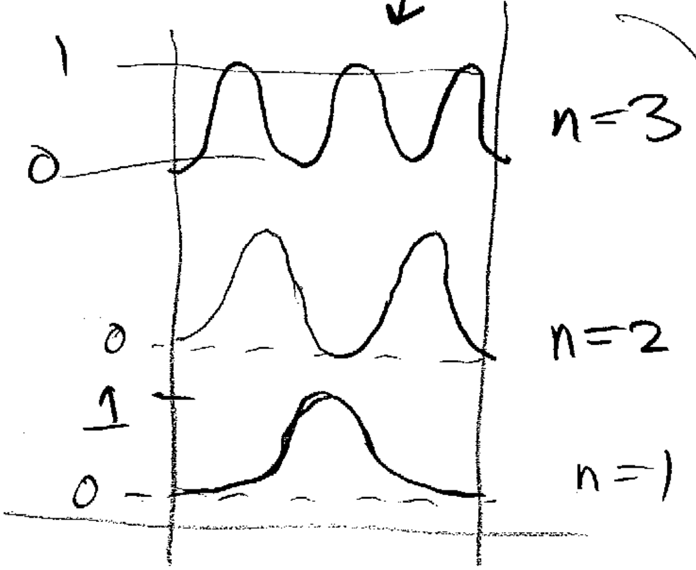
$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle$$

$$= \int_0^a dx \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \alpha\delta\left(x - \frac{a}{2}\right) \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right)$$

$$= \frac{2}{a}\alpha \int_0^a dx \, \underbrace{\sin^2\left(\frac{n\pi}{a}x\right)}_{\text{plot.}} \delta\left(x - \frac{a}{2}\right)$$

$\underline{1}$ if n is $\underline{\text{odd}}$.

0 if n is even.



meaning $E_n^1 = E_n^0 = \frac{n^2\pi^2\hbar^2}{2ma^2}$ $n =$ even

$= E_n^0 + \frac{2}{a}\alpha = \frac{n^2\pi^2\hbar^2}{2ma^2} + \frac{2}{a}\alpha$ $n =$ odd

only works when

$$\frac{2}{a}\alpha \ll \frac{\pi^2\hbar^2}{2ma^2}$$

end Lec #1

$$\alpha \ll \frac{\pi^2\hbar^2}{4ma^3}$$

$\boxed{\text{Step \#4}}$ get ψ_n^1

Retrace steps back to ...

$$\underline{H^0|\psi_n^1\rangle + H'|\psi_n^0\rangle = E_n^0|\psi_n^1\rangle + E_n^1|\psi_n^0\rangle}$$

"Bracket" not with $\langle\psi_n^0|$ but $\langle\psi_m^0|$,

where $m \neq n$

know but don't plug in ...

note: $\langle\psi_m^0|H^0|\psi_n^1\rangle$ $E_m^0 \underbrace{\langle\psi_m^0|\psi_n^1\rangle}_{\text{leave.}}$

leave $\langle\psi_m^0|H'|\psi_n^0\rangle$,

$E_n^0\langle\psi_m^0|\psi_n^1\rangle$

and $E_n^1\underbrace{\langle\psi_m^0|\psi_n^0\rangle}_{m\neq n} = 0$