Time independent nondegenerate perturbation theory

No hats

Goal: given H, find eigenstates & eigenvalue

$$\hat{H}\,|E_n\rangle = E_n\,|E_n\rangle$$

Suppose $\hat{H}$ is "close to" another hamiltonian $\hat{H}^0$ whose eigenstates & eigenvalues we already know

$$\hat{H}^0\,|E_n^0\rangle = E_n^0\,|E_n^0\rangle$$

$$\hat{H} = \hat{H}^0 + \lambda\hat{H}^1$$

$\hat{H}^0$ = exact Hamiltonian, unperturbed Hamiltonian

$\lambda\hat{H}^1$ = perturbation ("small")

Assumptions: $|E_n^0\rangle$ are nondegenerate

orthonormalized ~~Also~~ $\langle E_n^0|E_m^0\rangle = \delta_{nm}$

~~and~~ Also H^0 and $\hat{H}^1$ ~~are~~ independent of t

We will find $|E_n\rangle$ and E_n in a perturbation series in λ

$$|E_n\rangle = |E_n^0\rangle + \lambda|E_n^1\rangle + \lambda^2|E_n^2\rangle + \dots$$

$$E_n = E_n^0 + \underbrace{\lambda E_n^1}_{\text{first order correction}} + \underbrace{\lambda^2 E_n^2}_{\text{2nd order correction}} + \dots$$

$$(\hat{H}^0 + \lambda \hat{H}')(|E_n^0\rangle + \lambda |E_n^1\rangle + \lambda^2 |E_n^2\rangle + \dots)$$

$$= (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots)(|E_n^0\rangle + \lambda |E_n^1\rangle + \lambda^2 |E_n^2\rangle + \dots)$$

True for arbitrary λ so match powers of λ on either side

λ^0: $\hat{H}^0 |E_n^0\rangle = E_n^0 |E_n^0\rangle$ ✓

λ^1: $\hat{H}' |E_n^0\rangle + \hat{H}^0 |E_n^1\rangle = E_n^1 |E_n^0\rangle + E_n^0 |E_n^1\rangle$

λ^2: $\hat{H}' |E_n^1\rangle + \hat{H}^0 |E_n^2\rangle = E_n^2 |E_n^0\rangle + E_n^1 |E_n^1\rangle + E_n^0 |E_n^2\rangle$

$O(\lambda^1)$: Take inner product w/ $\langle E_m^0|$

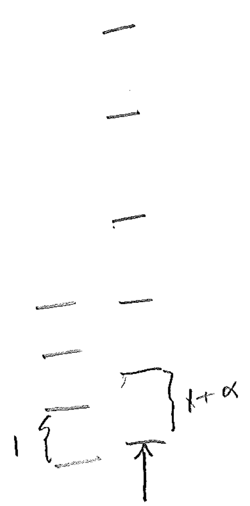
$$\langle E_m^0 | \hat{H}' | E_n^0\rangle + \underbrace{\langle E_m^0 | \hat{H}^0}_{\langle E_m^0 | E_m^0} | E_n^1\rangle = E_n^1 \underbrace{\langle E_m^0 | E_n^0\rangle}_{\delta_{mn}} + E_n^0 \langle E_m^0 | E_n^1\rangle$$

Consider $m = n \Rightarrow$ 2 terms cancel

$$\Rightarrow \boxed{E_n^1 = \langle E_n^0 | \hat{H}' | E_n^0\rangle} \quad \text{i.e.} \quad E_n = E_n^0 + \langle E_n^0 | \lambda \hat{H}' | E_n^0\rangle$$

anharmonic oscillator example: $H^0 =$ harmonic oscillator, where $V(x) = \frac{1}{2} m\omega^2 x^2$

let $\lambda H' = \lambda x^4 = \lambda \left(\frac{\hbar}{2m\omega}\right)^2 (a + a^\dagger)^4$



As we found earlier $\langle n | (a + a^\dagger)^4 | n\rangle$

$$= \langle n | \underbrace{aaa^\dagger a^\dagger}_{(n+1)(n+2)} + \underbrace{aa^\dagger aa^\dagger}_{(n+1)^2} + \underbrace{a^\dagger aaa^\dagger}_{n(n+1)} + \underbrace{aa^\dagger a^\dagger a}_{n(n+1)} + \underbrace{a^\dagger aa^\dagger a}_{n^2} + \underbrace{a^\dagger a^\dagger aa}_{(n-1)n} | n\rangle$$

$$= 6n^2 + 6n + 3$$

$$E_n^1 = \frac{3\hbar^2}{2m^2\omega^2}\lambda \left(n^2 + n + \tfrac{1}{2}\right) = \hbar\omega\, \alpha \left(\tfrac{1}{2} + n + n^2\right) \qquad \alpha = \frac{3\hbar\lambda}{2m^2\omega^3}$$

$$E_n^0 = \hbar\omega\left(\tfrac{1}{2} + n\right)$$

$$E_n = \hbar\omega\left(\tfrac{1}{2}(1+\alpha) + n(1+\alpha) + \alpha n^2\right)$$

(Note pt. breaks down for large n, why?)

shifts up ground state, increases spacing + makes spacing increase (~ ptcl in a box ~ λx^4)

$O(\lambda^1)$

Let $m \neq n$, then

$$\langle E_m^0 | \hat{H}' | E_n^0 \rangle + E_m^0 \langle E_m^0 | E_n^1 \rangle = E_n^0 \langle E_m^0 | E_n^1 \rangle$$

$$\langle E_m^0 | E_n^1 \rangle = \frac{\langle E_m^0 | \hat{H}' | E_n^0 \rangle}{E_n^0 - E_m^0} \quad \text{for } m \neq n$$

Now $|E_n^0\rangle$ is a complete basis so

$$|E_n^1\rangle = \sum_l c_{nl} |E_l^0\rangle$$

$$\langle E_m^0 | E_n^1 \rangle = \sum c_{nl} \langle E_m^0 | E_l^0 \rangle = c_{nm}$$

so

$$|E_n^1\rangle = c_{nn} |E_n^0\rangle + \sum_{m \neq n} c_{nm} |E_m^0\rangle$$

$$= c_{nn} |E_n^0\rangle + \sum_{m \neq n} |E_m^0\rangle \frac{\langle E_m^0 | \hat{H}' | E_n^0 \rangle}{E_n^0 - E_m^0}$$

What about c_{nn}? We can set it equal to zero so th

Technical details

$$1 = \langle E_n | E_n \rangle = \underbrace{\langle E_n^0 | E_n^0 \rangle}_{1} + \lambda \langle E_n^1 | E_n^0 \rangle + \lambda \langle E_n^0 | E_n^1 \rangle + O(\lambda^2)$$

$$\Rightarrow \langle E_n^1 | E_n^0 \rangle + \underbrace{\langle E_n^0 | E_n^1 \rangle}_{\langle E_n^1 | E_n^0 \rangle^*} = 0$$

so $c_{nn} = \langle E_n^1 | E_n^0 \rangle$ must be imaginary, call it $i\theta$

$$|E_n\rangle = |E_n^0\rangle + \lambda |E_n^1\rangle$$

$$= |E_n^0\rangle + i\lambda\theta |E_n^0\rangle + \lambda \sum |E_m^0\rangle \frac{\langle\ \rangle}{E_n^0 - E_m^0} + O(\lambda^2)$$

$$= e^{i\lambda\theta} |E_n^0\rangle + \lambda \sum |\ \rangle \frac{\langle\ \rangle}{E - E}$$

$$= e^{i\lambda\theta} \left(|E_n^0\rangle + \lambda \sum |\ \rangle \frac{\langle\ \rangle}{E - E} + O(\lambda^2) \right)$$

Thus by rescaling the phase

$$|E_n^1\rangle = |E_n^0\rangle + \sum_{m\neq n} \frac{|E_m^0\rangle\langle E_m^0|\lambda \hat{H}'|E_n^0\rangle}{E_n^0-E_m^0}$$

Note that as long as eigenstates are nondegenerate, the denominator does not go to zero
(otherwise need degenerate p.t.)

do examples

2nd order p.t. (if 1st order result vanishes)

Take inner product $O(\lambda^2)$ eqn w/ $\langle E_n^0|$

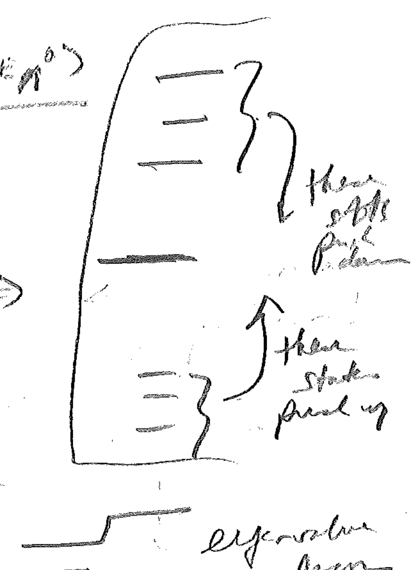
$$\langle E_n^0|\hat{H}'|E_n^1\rangle + \underbrace{\langle E_n^0|\hat{H}^0|E_n^2\rangle}_{E_n^0\langle E_n^0|E_n^2\rangle} = E_n^2 + E_n^1\langle E_n^0|E_n^1\rangle + E_n^0\langle E_n^0|E_n^2\rangle$$

cancel

$$E_n^2 = \langle E_n^0|\hat{H}'|E_n^1\rangle + E_n^1\underbrace{\langle E_n^0|E_n^1\rangle}_{\because\, c_{nn}=0}$$

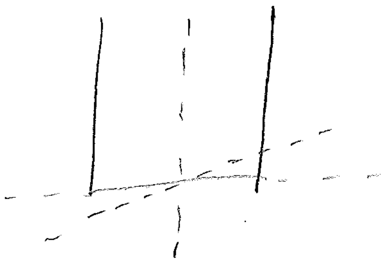
$$= \sum_{m\neq n}\frac{\langle E_n^0|\hat{H}'|E_m^0\rangle\langle E_m^0|\hat{H}'|E_n^0\rangle}{E_n^0-E_m^0}$$

$$E_n^2 = \sum_{m\neq n}\frac{|\langle E_n^0|\hat{H}'|E_m^0\rangle|^2}{E_n^0-E_m^0} \Rightarrow$$



- Near states affect E more than far states
- gnd state energy always goes down in 2nd order p.t.

If unperturbed potential is even, and perturbation is odd
then 1st order correction vanishes



$V^0(x)$ = particle in a box

$\lambda H' = qEx$

(eg charged particle in const field)

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

$$= \int_{-\infty}^{\infty} dx\, \underbrace{|u_n^0(x)|^2}_{\text{even}}\ \underbrace{qEx}_{\text{odd}} = 0$$

1st order correction to wavefunction may only have certain terms

eg. if $u_n^0(x)$ is even & H' is even
then only even terms are in correction

$$u_n^1(x) = u_n^0(x) + \sum \frac{u_m^0(x)}{E_n^0 - E_m^0} \int dx\, (u_m^0(x))^* \underbrace{\lambda H'(u_n^0(x))}_{\text{even}}$$

must be even

= only even terms