Physics 492
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Lecture #9 Perturbation theory

A systematic way of doing approximations in Q.M.
Begin with time independent theory.

$$\hat{H} = \hat{H}_0 + \lambda \hat{H}_1$$

- $\hat{H}_0$ has exact, known solutions
- $\hat{H}_1$ time independent.
- λ small bookkeeping parameter

For example, relativistic KE correction to Hydrogen

$$\lambda \hat{H}_1 = -\frac{1}{8} \frac{\hat{p}^4}{m^3 c^2}$$

no obvious λ but correction is proportional to α^4.

Expand wave function and energies as

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

$$\hat{H}|\psi_n\rangle = (\hat{H}_0 + \lambda \hat{H}_1)\left[|\psi_n^0\rangle + \lambda |\psi_n^1\rangle + \cdots\right]$$

$$= (E_n^0 + \lambda E_n^1 + \cdots)\left[|\psi_n^0\rangle + \lambda |\psi_n^1\rangle + \cdots\right]$$

Compare order by order in λ

$\mathcal{O}(\lambda^0)$ $\quad (\hat{H}_0 - E_n^0)|\psi_n^0\rangle = 0$

$\mathcal{O}(\lambda^1)$ $\quad (\hat{H}_0 - E_n^0)|\psi_n^1\rangle = (E_n^1 - \hat{H}_1)|\psi_n^0\rangle$

$\mathcal{O}(\lambda^2)$ $\quad (\hat{H}_0 - E_n^0)|\psi_n^2\rangle = (E_n^1 - \hat{H}_1)|\psi_n^1\rangle + E_n^2|\psi_n^0\rangle$

$\mathcal{O}(\lambda^3)$ $\quad (\hat{H}_0 - E_n^0)|\psi_n^3\rangle = (E_n^1 - \hat{H}_1)|\psi_n^2\rangle + E_n^2|\psi_n^1\rangle + E_n^3|\psi_n^0\rangle$

We see we can take $|\psi_n^k\rangle \longrightarrow |\psi_n^k\rangle + c|\psi_n^0\rangle$ and not change left side, thus not affecting result to order k. We are free to choose

$$\langle\psi_n^k|\psi_n^0\rangle = 0$$

This ensures $|\psi_n\rangle$ is normalized to first order in λ:

$$\langle\psi_n|\psi_n\rangle = \left(\langle\psi_n^0| + \langle\psi_n^1|\lambda + \cdots\right)\left(|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \cdots\right)$$

$$= 1 + \lambda\left(\langle\psi_n^1|\psi_n^0\rangle + \langle\psi_n^0|\psi_n^1\rangle\right) + \mathcal{O}(\lambda^2)$$

actually, we only need real part of $\langle\psi_n^1|\psi_0\rangle$ to be zero. let $\langle\psi_n^1|\psi_0\rangle = ia$

$$|\psi_n\rangle = |\psi_n^0\rangle + \lambda\left(|\psi_n^1\rangle + ia|\psi_n^0\rangle\right) + \mathcal{O}(\lambda^2)$$

$$= (1 + ia\lambda)|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \mathcal{O}(\lambda^2)$$

$$= e^{ia\lambda}|\psi_n^0\rangle + \lambda|\psi_n^1\rangle + \mathcal{O}(\lambda^2)$$

to this order in λ $\qquad$ an irrelevant phase

First order energy correction: $O(\lambda^1)$ equation and apply bra $\langle \psi_n^0|$

$$\langle \psi_n^0 | \underbrace{\hat{H}_0}_{E_n^0} - E_0 | \psi_n^1 \rangle = \langle \psi_n^0 | (E_n^1 - \hat{H}_1) | \psi_n^0 \rangle$$

$$E_n^1 = \langle \psi_n^0 | \hat{H}_1 | \psi_n^0 \rangle \equiv [\hat{H}_1]_{nn}$$

matrix element

First order wave function:

Expand $|\psi_n^1\rangle$ in terms of zeroth order wave function, with $\langle \psi_n^1 | \psi_n^0 \rangle = 0$

$$|\psi_n^1\rangle = \sum_{k \neq n} C_k |\psi_k^0\rangle$$

$$(\hat{H}^0 - E_n^0) \sum_{k \neq n} C_k |\psi_k^0\rangle = (E_n^1 - \hat{H}_1) |\psi_n^0\rangle$$

take inner product with $\langle \psi_\ell^0 |$ & $\langle \psi_\ell^0 | \hat{H}^0 = \langle \psi_\ell^0 | E_\ell^0$

$$\sum_{k \neq n} C_k (E_\ell^0 - E_n^0) \underbrace{\langle \psi_\ell^0 | \psi_k^0 \rangle}_{\delta_{\ell k}} = \langle \psi_\ell^0 | (E_n^1 - \hat{H}_1 | \psi_n^0 \rangle$$

$$C_\ell (E_\ell^0 - E_n^0) = E_n^1 \langle \psi_\ell^0 | \psi_n^0 \rangle - \langle \psi_\ell^0 | \hat{H}_1 | \psi_n^0 \rangle$$

for $\ell = n$ recover first order energy.

for $\ell \neq n$

$$C_\ell = \frac{\langle \psi_\ell^0 | \hat{H}_1 | \psi_n^0 \rangle}{E_n^0 - E_\ell^0} = \frac{[\hat{H}_1]_{\ell n}}{E_n^0 - E_\ell^0}$$

changing dummy index l back to k,

$$|\psi_n^1\rangle = \sum_{k\neq n} \frac{[\hat{H}_1]_{kn}}{E_n^0 - E_k^0} |\psi_k^0\rangle$$

Only works if unperturbed states are non-degenerate.

<u>2nd order energy</u> : $\mathcal{O}(\lambda^2)$ equation
act with bra $\langle\psi_n^0|$

$$0 = \langle\psi_n^0|(E_n^1 - \hat{H}_1)|\psi_n^1\rangle + E_n^2 \langle\psi_n^0|\psi_n^0\rangle$$

with $\langle\psi_n^0|\psi_n^1\rangle = 0$,

$$E_n^2 = \langle\psi_n^0|\hat{H}_1|\psi_n^1\rangle =$$

$$\sum_{k\neq n} \frac{\langle\psi_k^0|\hat{H}_1|\psi_n^0\rangle\langle\psi_n^0|\hat{H}_1|\psi_k^0\rangle}{E_n^0 - E_k^0}$$

$$= \sum_{k\neq n} \frac{|[\hat{H}_1]_{kn}|^2}{E_n^0 - E_k^0}$$

Some examples

<u>Example 1</u> perturbed 1D harmonic oscillator

$$\hat{H}_0 = \frac{\hat{P}_x^2}{2m} + \frac{1}{2} m\omega^2 \hat{x}^2$$

$$\lambda \hat{H}_1 = b\hat{x}^4$$

introduce ground state classical turning point

$$x_c = \sqrt{\frac{\hbar}{m\omega}}$$

$$\hat{y} \equiv \sqrt{\frac{m\omega}{\hbar}}\, \hat{x} = \frac{\hat{x}}{x_c} \ ; \quad \hat{q} \equiv \frac{\hat{p}}{\sqrt{m\omega\hbar}} = \frac{x_c}{\hbar}\hat{p}$$

$[\hat{y}, \hat{q}] = i$ let $\lambda = \dfrac{b x_c^4}{\hbar\omega}$ then

$$\boxed{\hat{H} = \frac{\hbar\omega}{2}\left(\hat{y}^2 + \hat{q}^2\right) + \lambda \hbar\omega\, \hat{y}^4}$$

define $\hat{a} \equiv \frac{1}{\sqrt{2}}(\hat{y} + i\hat{q})$; $[\hat{a}, \hat{a}^+] = 1$

$$\hat{y} = \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^+)$$

then
$$\hat{a}^+ |n\rangle = \sqrt{n+1}\, |n+1\rangle$$
$$\hat{a}\, |n\rangle = \sqrt{n}\, |n-1\rangle$$
$$\hat{a}^+\hat{a}\, |n\rangle = n\, |n\rangle$$

1^{st} order energy correction

$$\lambda E_n' = \lambda \hbar\omega \langle n|\hat{y}^4|n\rangle$$

$$\hat{y}^2 = \frac{1}{2}\left(\hat{a}^2 + \hat{a}^{+2} + \hat{a}\hat{a}^+ + \hat{a}^+\hat{a}\right) = \frac{1}{2}\left(\hat{a}^2 + \hat{a}^{+2} + 2\hat{a}^+\hat{a} + 1\right)$$

$$\hat{y}^2|n\rangle = \frac{1}{2}\Big\{\sqrt{n(n-1)}\,|n-2\rangle + \sqrt{(n+1)(n+2)}\,|n+2\rangle + (2n+1)|n\rangle\Big\}$$

$$\langle n|\hat{y}^2\hat{y}^2|n\rangle = \frac{1}{4}\left[n(n-1) + (n+1)(n+2) + (2n+1)^2\right]$$
$$= \frac{3}{4}\left(2n^2 + 2n + 1\right)$$

for perturbation theory to be valid $\lambda E_n' \ll E_n^0$

$$\lambda E_n' = \lambda\hbar\omega\left(\frac{3}{4}\right)(2n^2+2n+1) \;\overset{?}{\ll}\; \hbar\omega\left(n+\frac{1}{2}\right)$$

$$b\,x_c^4\left(\frac{3}{4}\right)(2n^2+2n+1) \;\overset{?}{\ll}\; \hbar\omega\left(n+\frac{1}{2}\right)$$

Since $\lambda E_n' \xrightarrow[n\to\infty]{} b x_c^4 \frac{3}{2} n^2$ & $E_n^0 \xrightarrow[n\to\infty]{} \hbar\omega n$ eventually perturbation theory breaks down:

$$n^2 > \frac{\hbar\omega}{b x_c^4}\left(\frac{2}{3}\right)$$

harmonic oscillator is a special case because $E_{n+1} - E_n = \hbar\omega$ independent of n.

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Example II linearly perturbed harmonic oscillator

$$\lambda \hat{H}' = -q\mathcal{E}\hat{x} = -q\mathcal{E}\sqrt{\frac{\hbar}{m\omega}}\,\hat{y} = -\hbar\omega\lambda\hat{y}$$

$\mathcal{E}$: electric field

$$\lambda = \frac{1}{\hbar\omega}\, q\mathcal{E}\sqrt{\frac{\hbar}{m\omega}}$$

Note λ is somewhat arbitrary dimensionless parameter but this choice corresponds to shift in y in exact solution. The solution to perturbed problem is independent of this choice.

$$\lambda E_n' = -\hbar\omega\lambda \langle n| \frac{1}{\sqrt{2}}(\hat{a} + \hat{a}^\dagger)|n\rangle = 0$$

first order correction vanishes.

However, in this case we can easily calculate the exact answer:

$$\hat{y}' \equiv \hat{y} - \lambda$$

$$\hat{y}'^2 = \hat{y}^2 - 2\lambda\hat{y} + \lambda^2$$

$$\hat{H} = \frac{1}{2}\hbar\omega\left(\hat{y}^2 + \hat{\varrho}^2 - 2\lambda\hat{y}\right) = \frac{1}{2}\hbar\omega\left(\hat{y}'^2 + \hat{\varrho}^2 - \lambda^2\right)$$

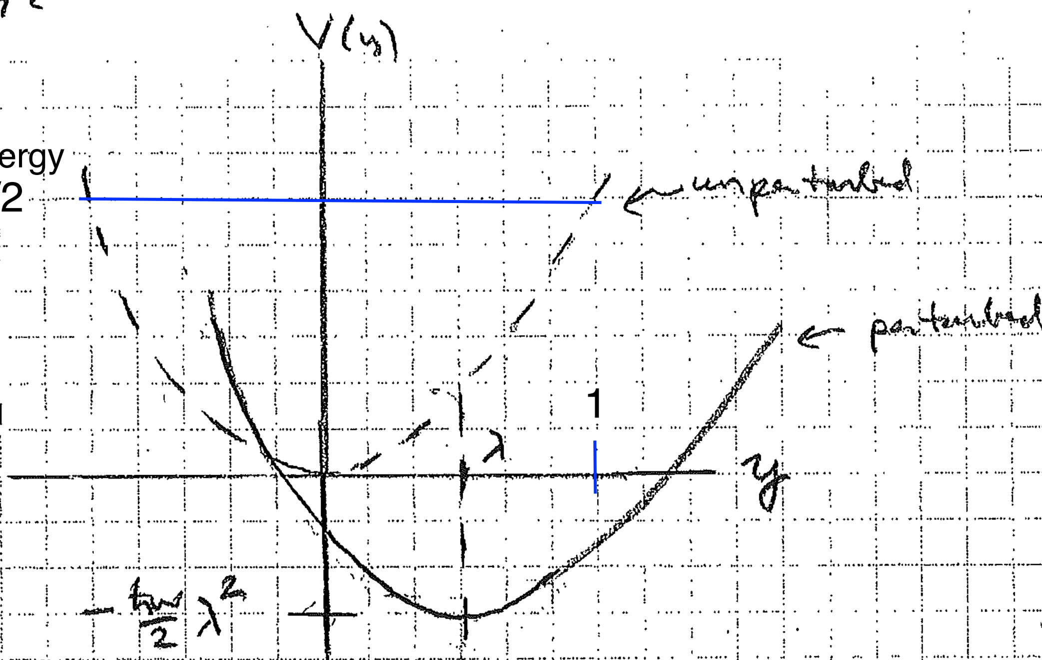
just a constant term added to the energy

since $[\hat{y}', \hat{\varrho}] = [\hat{y}, \hat{\varrho}] = i$

$$E_n = \hbar\omega\left[n + \frac{1}{2} - \frac{1}{2}\lambda^2\right]$$

ground state energy
$\hbar\omega/2$

Note: analogous to classical mass on a spring-- horizontal versus vertical in gravitational potential



oscillator with linear perturbation

exact answer has only λ^2 correction.

Second order perturbation theory should give exact energy:

$$\boxed{E_n^{(2)} = \sum_{k \neq n} \frac{|\langle \phi_k | \hat{H}_1 | \phi_n \rangle|^2}{E_n^0 - E_k^0}}$$

Note change of notation

$|\psi_n^0\rangle = |\phi_n\rangle$ here and $|\psi_n'\rangle = |\phi_n'\rangle$

2nd order energy correction

For $\lambda \hat{H}' = -\hbar\omega\lambda\hat{y}$ nonvanishing terms in sum come from $k = n \pm 1$

$$\langle n+1 | \tfrac{1}{\sqrt{2}}(\hat{a} + \hat{a}^+) | n \rangle = \sqrt{\frac{n+1}{2}}$$

$$\langle n-1 | \tfrac{1}{\sqrt{2}}(\hat{a} + \hat{a}^+) | n \rangle = \sqrt{\frac{n}{2}}$$

energy denominators:

$$E_n - E_{n+1} = -\hbar\omega$$

$$E_n - E_{n-1} = +\hbar\omega$$

$$\lambda^2 E_n^{(2)} = (\hbar\omega\lambda)^2 \left(\frac{\frac{n+1}{2}}{-\hbar\omega} + \frac{\frac{n}{2}}{\hbar\omega} \right) = -\frac{\hbar\omega\lambda^2}{2}$$

<u>perturbed wave function</u>

Exact solution $|n\rangle_\lambda = \hat{T}(\lambda)|n\rangle = e^{-i\lambda\hat{q}}|n\rangle$

first order correction is

$$|n\rangle_\lambda \cong (1 - i\lambda\hat{q})|n\rangle = |n\rangle \underbrace{-i\lambda\hat{q}|n\rangle}_{|\varphi_n^1\rangle}$$

$$-i\hat{q} = \frac{1}{\sqrt{2}}\left(\hat{a}^\dagger - \hat{a}\right)$$

so $\lambda|\varphi_n^1\rangle = -\lambda \frac{1}{\sqrt{2}}(\hat{a}^\dagger - \hat{a})|n\rangle = \frac{\lambda}{\sqrt{2}}\left(\sqrt{n+1}|n+1\rangle - \sqrt{n}|n-1\rangle\right)$

first order perturbation theory gives same answer -

$$\lambda|\varphi_n^1\rangle = \sum_{m \neq n} |m\rangle \frac{\langle m|\hat{H}_1|n\rangle}{E_n^0 - E_m^0} = -\lambda\hbar\omega \sum_{m \neq n} |m\rangle \frac{\langle m|\hat{q}|n\rangle}{E_n^0 - E_m^0}$$

$$= -\lambda\hbar\omega \left[|n+1\rangle \frac{\langle n+1|\hat{q}|n\rangle}{-\hbar\omega} + |n-1\rangle \frac{\langle n-1|\hat{q}|n\rangle}{+\hbar\omega} \right]$$

$$= \frac{\lambda}{\sqrt{2}} \left[\sqrt{n+1}|n+1\rangle - \sqrt{n}|n-1\rangle \right]$$

<u>Comment</u>

$$\lambda \hat{H}_1 = -Q\mathcal{E}\hat{x} = -Q\mathcal{E}x_c\hat{y}$$

$$\hat{H} = \frac{\hbar\omega}{2}\left(\hat{y}^2 + \hat{q}^2\right) - Q\mathcal{E}x_c\hat{y}$$

$$\hat{y}' = \hat{y} - \frac{Q\mathcal{E}x_c}{\hbar\omega} \quad \text{dimensionless shift}$$

$$(\hat{y}')^2 = \hat{y}^2 - 2\frac{Q\mathcal{E}x_c}{\hbar\omega}\hat{y} + \left(\frac{Q\mathcal{E}x_c}{\hbar\omega}\right)^2$$

$$\hat{H} = \frac{1}{2}\hbar\omega\left(\hat{y}'^2 + \hat{q}^2\right) - \frac{1}{2}\hbar\omega\left(\frac{Q\mathcal{E}x_c}{\hbar\omega}\right)^2$$

$$E_n^{exact} = \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right) - \frac{1}{2}\hbar\omega\left(\frac{Q\mathcal{E}x_c}{\hbar\omega}\right)^2$$

Suppose we had taken

dim. constant

$$\lambda \hat{H}_1 = -Q\mathcal{E}x_c\hat{y} \equiv -c\hbar\omega\lambda\hat{y}, \quad \lambda \equiv \frac{Q\mathcal{E}x_c}{c\hbar\omega}$$

$$\lambda^2 E_n^2 = \sum_{k\neq n}\frac{|\langle k|\lambda\hat{H}_1|n\rangle|^2}{E_n^0 - E_k^0} = +(\lambda c\hbar\omega)^2\left(\frac{-1}{2\hbar\omega}\right)$$

$$\boxed{\lambda c\hbar\omega = Q\mathcal{E}x_c}$$

$$E_n \doteq E_n^0 + \underset{0}{\underset{\shortparallel}{\lambda E_n^1}} + \lambda^2 E_n^2 = \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right) - \left(\frac{1}{2\hbar\omega}\right)(Q\mathcal{E}x_c)^2$$

$$= \frac{1}{2}\hbar\omega\left(n+\frac{1}{2}\right) - \frac{1}{2}\hbar\omega\left(\frac{Q\mathcal{E}x_c}{\hbar\omega}\right)^2$$

Choice of λ arbitrary, small dimensionless constant for book keeping of perturbation expansion.

Problem with degeneracy:

Look at $O(\lambda^1)$ equation

$$(\hat{H}_0 - E_n^0)|\psi_n^{(1)}\rangle = (E_n^1 - \hat{H}_1)|\psi_n^{(0)}\rangle$$

which wave function to use in case of degeneracy?

$$|\psi_n^{(1)}\rangle = \sum_{k \neq n} C_n |\psi_k^{(0)}\rangle$$

$$C_k = \frac{\langle \psi_k^0 | \hat{H}_1 | \psi_n^0 \rangle}{E_n^0 - E_k^0}$$

C_k undefined in case of degeneracies.