Lecture #9, Perturbation Theory

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

\[ H = H_0 + \lambda H_1 \]

- \( H_0 \) has exact, known solutions
- \( H_1 \) time independent
- \( \lambda \) small bookkeeping parameter

For example, relativistic KE correction to Hydrogen

\[ \lambda \hat{H}_1 = -\frac{1}{8} \frac{\hbar^2}{m^3 c^2} \]

no obvious \( \lambda \) but correction is proportional to \( \alpha^4 \).

Expand wave function and energy as

\[ |\psi_n\rangle = |\psi_0\rangle + \lambda (|\psi_1\rangle + \lambda^2 |\psi_2\rangle + \cdots) \]
\[ E_n = E_0 + \lambda E_1 + \lambda^2 E_2 + \cdots \]

\[ \hat{H} |\psi_n\rangle = (\hat{H}_0 + \lambda \hat{H}_1) \left[ |\psi_0\rangle + \lambda |\psi_1\rangle + \cdots \right] \]
\[ = (E_0 + \lambda E_1 + \cdots) \left[ |\psi_0\rangle + \lambda |\psi_1\rangle + \cdots \right] \]
Compare order by order in $\lambda$

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

$O(\lambda^1) \quad (\hat{H}_0 - E_n^0) | \Psi_n^1 \rangle = (E_n^1 - \hat{A}_n) | \Psi_n^0 \rangle$

$O(\lambda^2) \quad (\hat{H}_0 - E_n^0) | \Psi_n^2 \rangle = (E_n^2 - \hat{A}_n) | \Psi_n^1 \rangle + E_n^2 | \Psi_n^0 \rangle$

$O(\lambda^3) \quad (\hat{H}_0 - E_n^0) | \Psi_n^3 \rangle = (E_n^3 - \hat{A}_n) | \Psi_n^2 \rangle + E_n^3 | \Psi_n^1 \rangle + O(\lambda^4)$

We see we can take $| \Psi_n^k \rangle \rightarrow | \Psi_n^k \rangle + c | \Psi_n^0 \rangle$

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 just order in $\lambda$:

$\langle \Psi_n | \Psi_n \rangle = (\langle \Psi_n^0 | + \langle \Psi_n^1 | \lambda + \ldots \rangle (\langle \Psi_n^1 | + i \langle \Psi_n^0 | + \ldots \rangle \langle \Psi_n^1 | + \ldots \rangle$  

$= 1 + \lambda (\langle \Psi_n^0 | \Psi_n^0 \rangle + \langle \Psi_n^1 | \Psi_n^1 \rangle) + O(\lambda^2)$

Actually, we only need real part of $\langle \Psi_n^1 | \Psi_n^0 \rangle$ to be zero. Let $\langle \Psi_n^0 | \Psi_n \rangle = i \lambda$

$| \Psi_n \rangle = \lambda | \Psi_n^0 \rangle + \lambda (1 | \Psi_n^1 \rangle + i | \Psi_n^0 \rangle) + O(\lambda^2)$

$= (1 + i \lambda | \Psi_n^0 \rangle + \lambda | \Psi_n^1 \rangle + O(\lambda^2)$

$= e^{i \lambda \kappa} | \Psi_n^0 \rangle + \lambda | \Psi_n^1 \rangle + O(\lambda^2)$

to the order in $\kappa$ an irrelevant phase
First order energy correction: $O(\lambda^2)$ equation
and apply bra $\langle \psi_0 |$

$$
\langle \psi_0 | H_0 - E_0 | \psi_n' \rangle = \frac{\langle \psi_0 | (E_n' - H) | \psi_n \rangle}{E_n'}
$$

$$
E_n' = \langle \psi_n | H | \psi_n \rangle = [H]_{nn} \text{ matrix element}
$$

First order wave function:

Expand $|\psi_n'\rangle$ in terms of zeroth order wave function, with $\langle \psi_0 | \psi_n \rangle = 0$

$$
|\psi_n'\rangle = \sum_{k \neq n} C_k |\psi_k\rangle
$$

$$(H_0 - E_0) \sum_{k \neq n} C_k |\psi_k\rangle = (E_n' - H) |\psi_n\rangle$$

take inner product with $\langle \psi_0 | \langle \psi_0 | H' = \langle \psi_0 | E_0^0$

$$
\sum_{k \neq n} C_k (E_0^0 - E_n^0) \langle \psi_0 | \psi_k \rangle = \langle \psi_0 | (E_n' - H) | \psi_0 \rangle
$$

$$
C_n (E_0^0 - E_n^0) = E_n' \langle \psi_0 | \psi_n \rangle - \langle \psi_0 | H | \psi_n \rangle
$$

for $n=n$ recover first order energy.

for $k \neq n$

$$
C_k = \frac{\langle \psi_0 | H | \psi_k \rangle}{E_0^0 - E_n^0} = \frac{[H]_{kn}}{E_n^0 - E_k^0}
$$
changing dummy index \( l \) back to \( k \),

\[
|\Psi_n'\rangle = \sum_{k \neq n} \frac{[\hat{H},]_{kn}}{E_n^0 - E_k^0} |\Psi_k\rangle
\]

Only works if unperturbed states are non-degenerate.

2\textsuperscript{nd} order energy: \( O(2^2) \) equation

act with bra \( \langle \Psi_0^0 | \)

\[
o = \langle \Psi_0^n | (E_n^0 - \hat{H}) | \Psi_n'\rangle + E_n^0 \langle \Psi_0^0 | \Psi_0^n \rangle
\]

with \( \langle \Psi_0^n | \Psi_n'\rangle = 0 \),

\[
E_n^2 = \langle \Psi_0^n | \hat{H} | \Psi_n'\rangle = \sum_{k \neq n} \frac{\langle \Psi_0^n | \hat{H} | \Psi_0^k \rangle \langle \Psi_0^k | \hat{H} | \Psi_0^n \rangle}{E_n^0 - E_k^0}
\]

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

**Example 1** perturbed 1D harmonic oscillator

\[ \hat{H}_0 = \frac{\hat{p}^2}{2m} + \frac{1}{2} mw^2 \hat{x}^2 \]

\[ \Delta H_1 = bx^4 \]

Introduce ground state classical turning point

\[ x_c = \sqrt{\frac{\hbar}{mw}} \]

\[ \hat{y} = \sqrt{\frac{mw}{\hbar}} \hat{x} = \frac{\hat{x}}{x_c} \quad \hat{\partial} = \hat{p}/\hbar = \frac{x_c}{\hbar} \hat{\partial} \]

\[ \left[ \hat{\partial}, \hat{y} \right] = i \quad \text{let } \lambda = \frac{bx_c^4}{\hbar w} \quad \text{then} \]

\[ \hat{H} = \frac{\hbar w}{2} \left( \hat{y}^2 + \frac{\hat{\partial}^2}{x_c^2} \right) + \lambda \hbar w \hat{y}^4 \]

Define \( \hat{d} = \frac{1}{\sqrt{2}} (\hat{y} + i\hat{\partial}) \), \( [\hat{\partial}, \hat{d}] = 1 \)

\[ \hat{y} = \frac{1}{\sqrt{2}} (\hat{d} + \hat{d}^+) \]

Then

\[ \hat{d}^+ \mid n \rangle = \sqrt{n+1} \mid n+1 \rangle \]

\[ \hat{\partial} \mid n \rangle = \sqrt{n} \mid n-1 \rangle \]

\[ \hat{d}^+ \hat{d} \mid n \rangle = n \mid n \rangle \]
First order energy correction

\[ \lambda E_n' = \frac{1}{2} \hbar \omega \langle n | \hat{\mathcal{A}}^2 | n \rangle \]

\[ \hat{\mathcal{A}}^2 = \frac{1}{2} (\hat{\mathcal{A}}^2 + \hat{\mathcal{A}}^2 + \hat{\mathcal{a}}^2 + \hat{\mathcal{a}}^2) = \frac{1}{2} (\hat{\mathcal{a}}^2 + \hat{\mathcal{a}}^2 + 2 \hat{\mathcal{a}} \hat{\mathcal{a}} + 1) \]

\[ \langle n | \hat{\mathcal{A}}^2 | n \rangle = \frac{1}{2} \left\{ n(n-1) | n-2 \rangle + \sqrt{(n+1)(n+2)} | n+2 \rangle + (2n+1) | n \rangle \right\} \]

\[ \langle n | \hat{\mathcal{A}}^2 | n \rangle = \frac{1}{2} \left[ n(n-1) + (n+1)(n+2) + (2n+1)^2 \right] \]

\[ = \frac{3}{2} (2n^2 + 2n + 1) \]

For perturbation theory to be valid \( \lambda E_n' \ll E_n \)

\[ \lambda E_n' = \lambda \frac{1}{2} n(n-1) + \frac{3}{2} \lambda n^2 + \frac{3}{2} \lambda n \]

\[ \beta \lambda \left( \frac{3}{2} \right) \left( n^2 + 2n + 1 \right) \]

\[ \approx \beta \lambda \left( \frac{3}{2} \right) \left( n^2 + 2n + 1 \right) \]

\[ \approx \beta \lambda \left( \frac{3}{2} \right) \left( n^2 + 2n + 1 \right) \]

Since \( \lambda E_n' \rightarrow \beta \lambda \left( \frac{3}{2} \right) n^2 + E_n \rightarrow \text{thin n} \)

Eventually perturbation theory breaks down:

\[ h > \frac{\hbar \omega}{k} \left( \frac{2}{3} \right) \]

Harmonic oscillator is a special case because

\[ E_{n+1} - E_n = \hbar \omega \quad \text{independent of n.} \]
Example II  linearly perturbed harmonic oscillator

\[ H' = -\frac{1}{2} \epsilon \nabla^2 \psi - \frac{\sqrt{m_0}}{\hbar} \cdot \frac{1}{2} \sqrt{\hbar} \psi = -\frac{1}{2} \hbar \omega \psi \]

electric field

\[ \Delta E_n' = -\frac{1}{2} \frac{1}{\hbar} \lambda \langle n \left[ \frac{1}{\hbar} \left( \psi' + \psi'^* \right) \nabla \right] \rangle = 0 \]

first order correction vanishes.

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

\[ \psi' = \psi - \lambda \]

\[ \psi'^* = \psi^* - 2 \lambda \psi^* + \lambda^2 \]

\[ E' = \frac{1}{2} \hbar \omega \left( \overset{\vdash}{\psi}^2 + \overset{\vdash}{\psi}'^2 - 2 \lambda \overset{\vdash}{\psi}^2 \right) = \frac{1}{2} \hbar \omega \left( \overset{\vdash}{\psi}'^2 + \overset{\vdash}{\psi}'^2 - \lambda^2 \right) \]

just a constant term added to the energy, since 

\[ [\overset{\vdash}{\psi}', \overset{\vdash}{\psi}] = [\overset{\vdash}{\psi}', \overset{\vdash}{\psi}] = i \]

\[ E_n = \frac{\hbar \omega}{2} \left( n + \frac{1}{2} - \frac{1}{2} \lambda^2 \right) \]
Note: analogous to classical mass on a spring-- horizontal versus vertical in gravitational potential.

The oscillator with linear perturbation has an exact answer with only $2^2$ correction. Second order perturbation theory should give exact energy:

$$E_{n}^{(2)} = \sum_{k \neq n} \frac{|\langle \phi_{k} | H_{1} | \phi_{n} \rangle |^2}{E_{n}^{0} - E_{k}^{0}}$$

2nd order energy correction

For $aH_{1} = -\hbar \omega \hat{y}$, nonvanishing terms in sum come from $k = N \pm 1$.

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

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

Note change of notation $| \psi_{n}^{0} \rangle = | \phi_{n} \rangle$.
Energy denominator:

\[ E_n - E_{n+1} = -\frac{\hbar}{\lambda} \]

\[ E_n - E_{n-1} = \frac{\hbar}{\lambda} \]

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

Perturbed wave function

Exact solution \( |\Psi(\lambda)\rangle = e^{i/\lambda} \delta |n\rangle \)

First order correction \( \delta \)

\[ |\Psi (\lambda)\rangle = (1 - i \delta |n\rangle - (1 - i \delta |n\rangle) \]

\[ = \frac{1}{\hbar|n\rangle} \]

\[ \delta |n\rangle = -\lambda \frac{1}{\hbar} (\delta^* |n\rangle) \]

First order perturbation theory gives same answer:

\[ \lambda |\langle m | n\rangle = \sum_m \frac{\langle m | \delta^* | n\rangle}{E_n - E_m} \]

\[ = -\lambda \sum_m \frac{\langle m | \delta^* | n\rangle}{E_n - E_m} \]

\[ = -\frac{\hbar}{\lambda} \left[ \frac{1}{\hbar} + \frac{1}{\lambda} - \frac{\langle n+1 | \delta^* | n\rangle}{\hbar} \right] \]

\[ = \frac{\hbar}{\lambda^2} \left[ \frac{1}{\hbar} \langle n+1 | \delta^* | n\rangle - \frac{1}{\lambda} \right] \]