Lecture 10 - Perturbation Theory

Idea: write $H = H^0 + H'$

H^0 = Hamiltonian we can solve
H' = perturbation

To keep track of powers, write $H = H^0 + \lambda H'$
λ = artificial parameter, set to 1 in end

Expect eigenstates

$$\psi_n = \psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \dots$$

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots$$

Where $\psi_n^{(0)}$ is eigenstate of H^0 with energy $E_n^{(0)}$

$\psi_n^{(1)}, E_n^{(1)}$ = first order corrections
etc

Schrodinger says $H\psi_n = E_n \psi_n$

$$(H^0 + \lambda H')(\psi_n^{(0)} + \lambda \psi_n^{(1)} + \lambda^2 \psi_n^{(2)} + \dots)$$
$$= (E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \dots)(\psi_n^{(0)} + \lambda \psi_n^{(1)} + \dots)$$

Equate like powers of λ:

$$H^0 \psi_n^{(0)} + \lambda H^0 \psi_n^{(1)} + \lambda H' \psi_n^{(0)} + \dots$$

$$= E_n^{(0)} \psi_n^{(0)} + \lambda E_n^{(1)} \psi_n^{(0)} + \lambda E_n^{(0)} \psi_n^{(1)} + \dots$$

Zero order: $H^{0}\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)}$
- what we already know

First order:

$$H^{0}\psi_n^{(1)} + H'\psi_n^{(0)} = E_n^{(0)}\psi_n^{(1)} + E_n^{(1)}\psi_n^{(0)}$$

Can solve this for $E_n^{(1)}$ and $\psi_n^{(1)}$

Take inner product with $\psi_n^{(0)}$
[Multiply by $\psi_n^{(0)*}$ and integrate over all space]

$$\langle\psi_n^{(0)}|H^{0}|\psi_n^{(1)}\rangle + \langle\psi_n^{(0)}|H'|\psi_n^{(0)}\rangle$$

$$= E_n^{(0)}\langle\psi_n^{(0)}|\psi_n^{(1)}\rangle + E_n^{(1)}\langle\psi_n^{(0)}|\psi_n^{(0)}\rangle$$

Use $\langle\psi_n^{(0)}|H^{0} = E_n^{(0)}\langle\psi_n^{(0)}|$, so

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

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

First order energy shift is equal to expectation value of perturbation energy

Seems pretty intuitive to me.
Use this already in HW 5.11
(Helium problem)
Estimated interaction energy as $\langle\frac{e^2}{|r_1-r_2|}\rangle$,
got a reasonable answer.

To find $\psi_n^{(1)}$, write

$$* \quad [H^0 - E_n^{(0)}]\psi_n^{(1)} = -[H' - E_n^{(1)}]\psi_n^{(0)}$$

Can always use $\psi_n^{(0)}$'s as our basis.. generally that is the best thing to do.

So write $\psi_n^{(1)} = \sum_{m \neq n} c_m^{(n)} \psi_m^{(0)}$

a) Leave out $c_n^{(n)}$ term, since we are looking for correction to $\psi_n^{(0)}$ anyway
If we put it in, how would we distinguish it from $\psi_n^{(0)}$?

b) Notation ugly... I've be using parenthesis on $\psi_n^{(1)}$ to distinguish from $(\psi_n)'$
Griffiths doesn't, and puts parens on $c_m^{(n)}$ instead.
I'll start conforming to Griffiths.

$$\psi_n' = \sum_{m \neq n} c_m^{(n)} \psi_m^0$$

Plug into $(*)$

$$\sum_{m \neq n} c_m^{(n)} (E_m^0 - E_n^0)\psi_m^0 = -(H' - E_n')\psi_n^0$$

Take inner product with ψ_ℓ^0:

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_m^n \langle \psi_\ell^0 | \psi_m^0 \rangle = -\langle \psi_\ell^0 | H' | \psi_n^0 \rangle + E_n' \langle \psi_\ell^0 | \psi_n^0 \rangle$$

Since $\langle \psi_\ell^0 | \psi_m^0 \rangle = \begin{cases} 0 & \text{for } \ell \neq m \\ 1 & \text{for } \ell = m \end{cases}$

get rid of sum

$$(E_\ell^0 - E_n^0)\, c_\ell^{(n)} = -\langle \psi_\ell^0 | H' | \psi_n^0 \rangle + E_n^1 \langle \psi_\ell^0 | \psi_n^0 \rangle$$

If $\ell = n$, get back to

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle$$ (no $c_n^{(n)}$ to worry about anyway)

If $\ell \neq n$, then $\langle \psi_\ell^0 | \psi_n^0 \rangle$ goes away

Get $$\boxed{c_\ell^{(n)} = \frac{\langle \psi_\ell^{(0)} | H' | \psi_n^0 \rangle}{E_n^0 - E_\ell^0}}$$

Say that perturbation "mixes in" other states

Get more mixing of states nearby in energy, where $E_n^0 - E_\ell^0$ is small