

# Perturbation theory

Read McIntyre 10.3-10.4

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# From last time:

Need to solve:  $H|n\rangle = E_n |n\rangle$  where  $H = H_0 + \lambda H'$

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

State:  $|n\rangle = |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \dots$

The solution to the unperturbed problem is known:

$$H_0 |n^{(0)}\rangle = E_n^{(0)} |n^{(0)}\rangle$$

$\langle k^{(0)} | n^{(0)} \rangle = \delta_{kn}$  - unperturbed states are orthogonal and form a complete basis:  $\sum_n |n^{(0)}\rangle \langle n^{(0)}| = 1$

Consider non-degenerate case: all  $E_n^{(0)}$  are different !

Find first- and second-order energy corrections and first-order state correction

# From last time:

## First-order energy correction

$$E_n^{(1)} = \left\langle n^{(0)} \left| H' \right| n^{(0)} \right\rangle$$

First-order energy correction = expectation value  
of the perturbation with respect to unperturbed states

Now looking for the first-order correction to the state

# From last time:

Collect terms which have the same perturbation order  $\lambda$ , in this case  $\lambda^1$  :

$$\left(H_0 - E_n^{(0)}\right) |n^{(1)}\rangle = \left(E_n^{(1)} - H'\right) |n^{(0)}\rangle$$

Multiply by  $\langle k^{(0)}|$ :

$$\langle k^{(0)}| \left(H_0 - E_n^{(0)}\right) |n^{(1)}\rangle = \langle k^{(0)}| \left(E_n^{(1)} - H'\right) |n^{(0)}\rangle$$

Important:  $k \neq n$

$$\langle k^{(0)}| \left(E_k^{(0)} - E_n^{(0)}\right) |n^{(1)}\rangle = \langle k^{(0)}| \left(E_n^{(1)} - H'\right) |n^{(0)}\rangle$$

# From last time:

$$\langle k^{(0)} | (E_k^{(0)} - E_n^{(0)}) | n^{(1)} \rangle = \langle k^{(0)} | (E_n^{(1)} - H') | n^{(0)} \rangle$$

LHS:  $(E_k^{(0)} - E_n^{(0)}) \langle k^{(0)} | n^{(1)} \rangle$

RHS:

$$\begin{aligned} \langle k^{(0)} | (E_n^{(1)} - H') | n^{(0)} \rangle &= E_n^{(1)} \langle k^{(0)} | n^{(0)} \rangle - \langle k^{(0)} | H' | n^{(0)} \rangle = \\ &= - \langle k^{(0)} | H' | n^{(0)} \rangle = -H'_{kn} \end{aligned}$$

$$\langle k^{(0)} | n^{(1)} \rangle = \frac{H'_{kn}}{(E_n^{(0)} - E_k^{(0)})}$$

Next: how to use this information to get  $|n^{(1)}\rangle$  ?

## First-order correction to the state

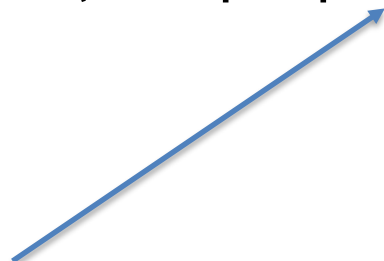
$$|n^{(1)}\rangle = \sum_{k \neq n} \frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle$$

$$H'_{kn} = \langle k^{(0)} | H' | n^{(0)} \rangle \text{ (matrix element of the perturbation)}$$

1. The first-order correction mixes states – the correction is a superposition of multiple states !
2. If  $H'_{kn} \neq 0$ , the highest contribution to the correction is from adjacent energy states

## Second-order correction to the energy

$$E_n^{(2)} = \langle n^{(0)} | H' | n^{(1)} \rangle = \sum_{k \neq n} \frac{|H'_{kn}|^2}{(E_n^{(0)} - E_k^{(0)})}$$


$$|n^{(1)}\rangle = \sum_{k \neq n} \frac{H'_{kn}}{(E_n^{(0)} - E_k^{(0)})} |k^{(0)}\rangle$$

# Things to note

1. When there is an off-diagonal term in the perturbation Hamiltonian (i.e.  $H'_{kn}$ ), there are first order corrections to the state/wave function.
2. Nearby (in energy) states "mix in" to a larger degree than far-away ones
3. Degeneracy presents problems in this formulation – denominator blows up (need new strategy)
4. "Small" means that off-diagonal matrix element is small relative to energy separations