Perturbation theory

Read McIntyre 10.3-10.4

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From last time:

Need to solve: $H|n> = En\,|n>$ *where* $H = H_0 + \lambda H'$

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

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

The solution to the unperturbed problem is known:

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

$\langle k^{(0)}|n^{(0)}\rangle = \delta_{kn}$ - 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

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

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 λ, in this case λ^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 ≠ 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:

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

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

RHS:

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

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

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

First-order correction to the state

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

$H'_{kn} = \langle k^{(0)}|H'|n^{(0)}\rangle$ (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

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

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

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