PERTURBATION THEORY (TIME-INDEPENDENT) 2

Problem: we have an Hamiltonian H^0 of which we know all eigenstates ψ_n^0 and eigenvalues E_n^0 that solve Schroedinger's equation:

$$H^0 \psi_n^0 = E_n^0 \psi_n^0$$

We perturb the Hamiltonian by adding a term $\lambda H'$ to it, and ask ourselves what we can say about the eigenstates ψ_n and eigenvalues E_n of $H = H^0 + \lambda H'$

Let us write ψ_n and E_n as a power series in λ:

$$\psi_n = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \ldots$$
$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \ldots$$

We can now use those expansion in the Schroedinger's equation $H\psi_n = E_n \psi_n$ and collect terms with the same power of λ. The terms multiplied by λ form the equation:

$$H^0 \psi_n^1 + H' \psi_n^0 = E_n^0 \psi_n^1 + E_n^1 \psi_n^0$$

From the above equation we derive:

$$E_n^1 = \langle \psi_n^0 | H' | \psi_n^0 \rangle$$

first-order correction to energy is expectation value of perturbation on unperturbed states

What can we say about the first-order correction on the wavefunction ψ_n^1?

Let us exploit the fact that the ψ_m^0 form a <u>complete</u> set: this means that any state can be written as a linear combination of ψ_m^0. In particular:

$$\psi_n^1 = \sum_m c_m^{(n)} \psi_m^0$$

Completeness and orthonormality also mean that :

$$\sum_n |\psi_n^0\rangle\langle\psi_n^0| = \mathbb{1} \quad : \text{ the identity operator}$$

Easy to prove :

completeness: any generic $|\psi\rangle$ can be written as $\sum_n c_n|\psi_n^0\rangle$

orthonormality: $\langle\psi_n^0|\psi_m^0\rangle = \delta_{nm}$ (Kronecker delta: $=1$ if $n=m$, $=0$ if $n\neq m$)

Then :

$$\underline{\underline{|\psi\rangle}} = \sum_n c_n|\psi_n^0\rangle = \sum_n c_n \overbrace{\sum_m |\psi_m^0\rangle\langle\psi_m^0|}^{\text{I insert this expression}}\psi_n^0\rangle =$$

$$= \sum_n c_n \sum_m \delta_{nm}|\psi_m^0\rangle = \sum_m |\psi_m^0\rangle \sum_n \delta_{nm} c_n =$$

$$= \sum_m c_m|\psi_m^0\rangle$$ same as above (m is just the name of the index in the sum)

$$= \underline{\underline{|\psi\rangle}}$$

Let us now go back to our expression:

$$H^0\psi_n^1 + H'\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0$$

$$H^0|\psi_n^1\rangle + H'|\psi_n^0\rangle = E_n^0|\psi_n^1\rangle + E_n^1|\psi_n^0\rangle$$

$$\Downarrow$$

$$\sum_m c_m^{(n)} H^0|\psi_m^0\rangle + H'|\psi_n^0\rangle = E_n^0\sum_m c_m^{(n)}|\psi_m^0\rangle + E_n^1|\psi_n^0\rangle$$

use $|\psi_n^1\rangle = \sum_m c_m^{(n)}|\psi_m^0\rangle$ use $|\psi_n^1\rangle = \sum_m c_m^{(n)}|\psi_m^0\rangle$

But $H^0|\psi_m^0\rangle = E_m^0|\psi_m^0\rangle$: $|\psi_m^0\rangle$ are solution of unperturbed H^0.

Therefore :

$$\sum_m c_m^{(n)}\overset{\text{numbers}}{(E_m^0 - E_n^0)}|\psi_m^0\rangle = -\overset{\text{operator}}{H'}|\psi_n^0\rangle + \overset{\text{number}}{E_n^1}|\psi_n^0\rangle$$

Let us also point out that we can <u>choose</u> $C_n^{(n)}$ to be equal to $\underline{\underline{\phi}}$.
$C_n^{(n)}$ tells us about the component along $|\psi_n^0\rangle$ of $|\psi_n^1\rangle$.
The equation that ψ_n^1 needs to solve is:

$$H^0\psi_n^1 + H^1\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0$$

Let us rewrite it:

$$(H^0 - E_n^0)\psi_n^1 = -(H^1 - E_n^1)\psi_n^0$$

Since $(H^0 - E_n^0)\psi_n^0 = 0$ [ψ_n^0 solves the Schroedinger's equation of the unperturbed system], if ψ_n^1 solves the equation above, also $\psi_n^1 + \alpha\psi_n^0$ does, for <u>any</u> value of α : I can use this freedom to <u>choose</u> $C_n^{(n)} = 0$.

Then, I can write:

$$\sum_{m\neq n} C_m^{(n)}(E_m^0 - E_n^0)|\psi_m^0\rangle = -H^1|\psi_n^0\rangle + E_n^1|\psi_n^0\rangle$$

Let us take the inner product with $\langle\psi_\ell^0|$:

$$\sum_{m\neq n} C_m^{(n)}(E_m^0 - E_n^0)\langle\psi_\ell^0|\psi_m^0\rangle = -\langle\psi_\ell^0|H^1|\psi_n^0\rangle + E_n^1\langle\psi_\ell^0|\psi_n^0\rangle$$

$\ell = n$: $$\sum_{m\neq n} C_m^{(n)}(E_m^0 - E_n^0)\delta_{nm} = -\langle\psi_n^0|H^1|\psi_n^0\rangle + E_n^1$$

ah, but $E_n^1 = \langle\psi_n^0|H^1|\psi_n^0\rangle$: $\phi = \phi$!

$\ell \neq n$: $$\sum_{m\neq n} C_m^{(n)}(E_m^0 - E_n^0)\delta_{\ell m} = -\langle\psi_\ell^0|H^1|\psi_n^0\rangle$$

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

$$\Rightarrow \boxed{C_\ell^{(n)} = \frac{\langle\psi_\ell^0|H^1|\psi_n^0\rangle}{E_n^0 - E_\ell^0}} \quad \text{and} \quad \boxed{\psi_n^1 = \sum_{m\neq n} \frac{\langle\psi_m^0|H^1|\psi_n^0\rangle}{E_n^0 - E_m^0}\psi_m^0}$$