Lecture 19: Perturbation theory: time-independent perturbations

Let us assume we have a non-degenerate system with an hamiltonian which consists of two parts:

$$H = H_0 + H' \tag{1}$$

whereby the dynamics induced by H_0 is fully solved and H' is a small perturbation to the system. The Schrödinger equation is given by:

$$H\psi = (H_0 + H')\psi = E\psi \tag{2}$$

with the problem:

$$H_0\psi_n^{(0)} = E_n^{(0)}\psi_n^{(0)} \tag{3}$$

being fully solved. In this case, we would say that H' is a perturbation to the Hamiltonian H_0. If ψ is a generic wavefunction, we can always express it as a linear combination of ψ_n:

$$\psi = \sum_m c_m\psi_m \tag{4}$$

Eq. 2 can thus be written as:

$$\sum_m c_m(E_m^{(0)} + H')\psi_m = \sum_m c_m E\psi_m \tag{5}$$

If we project onto one of the eigenfunctions of H_0, say ψ_k, we obtain:

$$c_k E_k^{(0)} + \sum_m c_m H'_{km} = E c_k \tag{6}$$

which is still an exact equation.

Let us study the correction to the wavefunction and its energy at the first order:

$$E \approx E^{(0)} + E^{(1)} \tag{7}$$

and

$$c_m \approx c_m^{(0)} + c_m^{(1)} \tag{8}$$

Substituting these two into Eq. 6:

$$(c_k^{(0)} + c_k^{(1)})E_k^{(0)} + \sum_m (c_m^{(0)} + c_m^{(1)})H'_{km} \approx (E^{(0)} + E^{(1)})(c_k^{(0)} + c_k^{(1)}) \tag{9}$$

At the zeroth order we have:

$$c_k^{(0)}(E_k^{(0)} - E^{(0)} = 0 \tag{10}$$

which trivially implies $E^{(0)} = E_n^{(0)}$.

At the first order we have instead:

$$c_k^{(1)} E_k^{(0)} + \sum_m c_m^{(0)} H'_{km} = E_n^{(0)} c_k^{(1)} + E^{(1)} c_k^{(0)} \tag{11}$$

For $k = n$ this translates into:

$$E^{(1)} = H'_{nn} = \langle \psi_n | H' | \psi_n \rangle \tag{12}$$

This is the first fundamental result in perturbation theory:

The correction at the first order in energy due to H' is simply the mean value of it over the same wavefunction.

Without demonstration, the correction at the first order to the wavefunction is:

$$\psi_n \approx \psi_n^{(0)} + \Sigma'_k \frac{H'_{kn}}{E_n^{(0)} - E_k^{(0)}} \psi_k^{(0)} \tag{13}$$