Time independent perturbations

(Bound state perturbation theory)

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Example:

He^+ (singly ionised Helium)

is a "Bohr-like" system with charge

$$\frac{(e)(-e)}{4\pi\epsilon_0} \rightarrow \frac{(2e)(-e)}{4\pi\epsilon_0}$$

The spetrum of eigenvalues is known.

Then treat neutral He atom as if the interaction between the two electrons is a "perturbation" (= small modification)

of the He^+ problem
i.e. think of the Hamiltonian

$$H = H_0 + \lambda V$$

where H_0 is a Hamilton whose eigenvalues and eigenvectors are completely known.

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

λV is called perturbing potential. Here λ is a real number, assumed $\ll 1$ and we make Taylor expansion of the ~~Bdl~~ correct energy eigenvalues E_n in parameter λ.

$$(H_0 + \lambda V)|n\rangle_\lambda = E_n^{(\lambda)} |n\rangle_\lambda$$

where $|n\rangle_\lambda$ are the eigen~~values~~ vectors of H

Now consider writing

$$E_n^{(\lambda)} = E_n^{(0)} + \lambda \Delta E_n^{(\lambda)} \quad ; \quad |n\rangle_\lambda = |n^{(0)}\rangle + \lambda |\Delta n\rangle_\lambda$$

Thus

$$(H_0 + \lambda V)(|n^{(0)}\rangle + \lambda |\Delta n\rangle_\lambda) = (E_n^{(0)} + \lambda \Delta E_n^{(\lambda)})(|n^{(0)}\rangle + \lambda |\Delta n\rangle_\lambda)$$

$$\underline{H_0 |n^{(0)}\rangle} + \lambda V |n^{(0)}\rangle + \lambda H_0 |\Delta n\rangle_\lambda + \lambda^2 V |\Delta n\rangle_\lambda$$
$$= \underline{E_n^{(0)} |n^{(0)}\rangle} + \lambda \Delta E_n^{(\lambda)} |n^{(0)}\rangle + \lambda E_n^{(0)} |\Delta n\rangle_\lambda + \lambda^2 \Delta E_n^{(\lambda)} |\Delta n\rangle_\lambda$$

$$V|n^{(0)}\rangle + H_0|\Delta n\rangle_\lambda = \Delta E_n^{(\lambda)}|n^{(0)}\rangle + E_n^{(0)}|\Delta n\rangle_\lambda$$

$$\boxed{(H_0 - E_n^{(0)})|\Delta n\rangle_\lambda = (\Delta E_n^{(\lambda)} - V)|n^{(0)}\rangle} \quad (1)$$

Both sides contains some unknowns and we need to solve this by some scheme

First note if we multiply by $\langle n^{(0)}|$ on the left,

$$\langle n^{(0)}|(H_0 - E_n^{(0)})|\Delta n\rangle_\lambda = 0$$

$$\therefore \Delta E_n^{(\lambda)} \underbrace{\langle n^{(0)}|n^{(0)}\rangle}_{=1} = \langle n^{(0)}|V|n^{(0)}\rangle$$

$$\therefore \boxed{\Delta E_n^{(\lambda)} = \langle n^{(0)}|V|n^{(0)}\rangle} \quad (2)$$

... valid to first order in λ

comment

$E_n^{(0)} \equiv E_n^{(0)} 1\!\!1$

Hilbert space identity operator

Thus the idea is to solve eq. (1) by an "iterative" procedure :

Take the answer from (2) for $\Delta E_n^{(\lambda)}$ and substitute in eq (1) R.H. Side

Then expect to solve for $|\Delta n\rangle_\lambda$ to the same level of accuracy, i.e. first order in λ

Thus schematically,

$$|\Delta n\rangle_\lambda = (H_0 - E_n^{(0)})^{-1} (\Delta E_n^{(\lambda)} - V) |n^{(0)}\rangle$$

But note that $(H_0 - \mathbb{1} E_n^{(0)})$ is an operator with eigenvalue 0 on $|n^{(0)}\rangle$

Thus $(H_0 - \mathbb{1} E_n^{(0)})$ does not have an inverse.

We will find a more restricted operator such that the zero eigenvalue eigenvector has been deleted from the list.

This restricted operator can then be inverted

<u>Basic idea</u>

$$\text{“}\frac{\mathbb{1}}{H_0 - E_n^{(0)}\mathbb{1}}\text{”} \equiv \text{“}\sum_k \frac{|k^{(0)}\rangle\langle k^{(0)}|}{H_0 - E_n^{(0)}\mathbb{1}}\text{”}$$

$$\xrightarrow{\text{modify to}} \sum_{k\neq n}{}' \frac{|k^{(0)}\rangle\langle k^{(0)}|}{H_0 - E_n^{(0)}\mathbb{1}}$$