Chapter 17 Perturbation Theory (Time-independent)

17.1. Formalism

A typical problem arising in physics is that, when trying to understand a system, you first make a very simple toy-model that you can solve exactly but that still captures the essential physics, and then, as you try to make the description more realistic, you add additional terms whose effects are smaller but still need to be taken into account for quantitative predictions.

In this case you can hope to be able to consider the additional terms as "small perturbations" and expand your observables as a power series in the perturbation, with rapid convergence.

We write the "toy-model" Hamiltonian as $\hat{H}_0$ and the "small" additional interaction as $\hat{H}_I$:

$$\hat{H} = \hat{H}_0 + \hat{H}_I \qquad \begin{array}{l} \hat{H}_0 = \text{"unperturbed Hamiltonian"} \\ \hat{H}_I = \text{"perturbation"} \end{array}$$

We know the eigenstates and eigenenergies of $\hat{H}_0$:

$$\hat{H}_0 |E_n^0\rangle = E_n^0 |E_n^0\rangle \equiv E_n^0 |n^0\rangle$$

We want the solutions of the full problem:

$$\hat{H}|n\rangle = E_n |n\rangle$$

We expand $\qquad E_n = E_n^0 + E_n^1 + E_n^2 + \ldots$

$$|n\rangle = |n^0\rangle + |n^1\rangle + |n^2\rangle + \dots$$

where, if we replace $\hat{H}_I$ by $\lambda \hat{H}_I$, these expansions show the following scaling with λ:

$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \dots$$

$$|n\rangle = |n^0\rangle + \lambda |n^1\rangle + \lambda^2 |n^2\rangle + \dots$$

Such that, in the limit $\lambda \to 0$, $E_n \to E_n^0$ and $|n\rangle \to |n^0\rangle$.

Terms of order λ^k are "k-th order terms" or "k-th order corrections", indicated by the superscript k. (E_n^k, $|n^k\rangle$).
With this counting, $\hat{H}_I$ is a first-order term, $\hat{H}_I \equiv \hat{H}^1$, while $\hat{H}_0 \equiv \hat{H}^0$ is of zeroth order.
A product like $E_n^k |n^{k'}\rangle$ would be of order $k+k'$.

The perturbative approach works if E_n^k and $\langle n^k | n^k \rangle$ get systematically smaller with increasing k at a rate such that the series converges. If that is the case, we call $\hat{H}_I$ a "small perturbation".

We can make almost any perturbation $\hat{H}_I$ small by multiplying it with $\lambda \ll 1$. We can then work out the series and sum it up. The key question is, of course, whether, when we later increase $\lambda \to 1$, the sum converges to a finite limit.

So we have

$$\left(\hat{H}^0 + \lambda \hat{H}^1\right)\left(|n^0\rangle + \lambda |n^1\rangle + \lambda^2 |n^2\rangle \cdots\right)$$
$$= \left(E_n^0 + \lambda E_n^1 + \lambda E_2^2 + \ldots\right)\left(|n^0\rangle + \lambda |n^1\rangle + \lambda^2 |n^2\rangle + \ldots\right) \qquad (*)$$

This has to hold not just at $\lambda = 1$, but any λ.

- Collecting terms of order 0 (i.e. without any factors of λ) we find

$$\boxed{\hat{H}^0 |n^0\rangle = E_n^0 |n^0\rangle}$$

i.e. the already solved unperturbed problem.

- Since $(*)$ holds for any λ, the term linear in λ have to balance separately:

$$\boxed{\hat{H}^0 |n^1\rangle + \hat{H}^1 |n^0\rangle = E_n^0 |n^1\rangle + E_n^1 |n^0\rangle}$$

Let us take the inner product with $\langle n^0|$. Using $\langle n^0|\hat{H}^0 = \langle n^0| E_n^0$ and $\langle n^0|n^0\rangle = 1$, we find

$$\cancel{\langle n^0|\hat{H}^0|n^1\rangle} + \langle n^0|\hat{H}^1|n^0\rangle = \cancel{\langle n^0|E_n^0|n^1\rangle} + E_n^1 \underbrace{\langle n^0|n^0\rangle}_{1}$$

$$\Rightarrow \quad \boxed{E_n^1 = \langle n^0|\hat{H}^1|n^0\rangle}$$

$\Rightarrow$ The first order correction in energy is the expectation value of $\hat{H}^1$ in the unperturbed state.

Now dot the equation with $\langle m^0|$ $(m \neq n)$:

$$\underbrace{\langle m^0|\hat{H}^0|n^1\rangle}_{E_m^0 \langle m^0|n^1\rangle} + \langle m^0|\hat{H}^1|n^0\rangle = E_n^0 \langle m^0|n^1\rangle$$

$$\Rightarrow \quad \boxed{\langle m^0|n^1\rangle = \frac{\langle m^0|\hat{H}|n^0\rangle}{E_n^0 - E_m^0}} \qquad \forall\, m \neq n$$

This determines all components of $|n'\rangle$ in the unperturbed energy eigenbasis, except for the component parallel to $|n^\circ\rangle$, $|n'_\parallel\rangle = |n^\circ\rangle\langle n^\circ|n'\rangle$.

To get $|n'_\parallel\rangle$ we demand that $|n\rangle$ is normalized up to terms of order λ^2:

$$1 = \langle n|n\rangle = \left(\langle n^\circ| + \lambda\langle n'_\perp| + \lambda\langle n'_\parallel|\right)\left(|n^\circ\rangle + \lambda|n'_\perp\rangle + \lambda|n'_\parallel\rangle\right)$$

$$= \underbrace{\langle n^\circ|n^\circ\rangle}_{1} + \lambda\langle n'_\parallel|n^\circ\rangle + \lambda\langle n^\circ|n'_\parallel\rangle + O(\lambda^2)$$

(since $\langle n'_\perp|n^\circ\rangle = 0$)

$$\Rightarrow \langle n^\circ|n'_\parallel\rangle + \underbrace{\langle n'_\parallel|n^\circ\rangle}_{=\langle n^\circ|n'_\parallel\rangle^*} = 0 \quad \text{up to terms of order } \lambda^2$$

$$\Rightarrow \langle n^\circ|n'_\parallel\rangle = i\alpha \quad (\text{pure imaginary, } \alpha\in\mathbb{R})$$

$$\Rightarrow |n\rangle = |n^\circ\rangle\langle n^\circ|n\rangle + \sum_{m\neq n}|m^\circ\rangle\langle m^\circ|n\rangle$$

$$= |n^\circ\rangle\langle n^\circ|\big(|n^\circ\rangle + \lambda\underbrace{|n'\rangle}_{\lambda|n'_\parallel\rangle+\lambda|n'_\perp\rangle}\big) + \sum_m{}' |m^\circ\rangle\langle m^\circ|\big(|n^\circ\rangle + \lambda|n'\rangle\big) + O(\lambda^2)$$

$$= |n^\circ\rangle\underbrace{\left(1 + \lambda i\alpha\right)}_{e^{i\lambda\alpha}+O(\lambda^2)} + \sum_m{}' |m^\circ\rangle\frac{\langle m^\circ|\lambda\hat{H}'|n^\circ\rangle}{E_n^0 - E_m^0} \quad \text{(from previous page, bottom)}$$

We can absorb the phase $e^{i\lambda\alpha}$ in the state $|n\rangle$ (which is ambiguous by a phase), by multiplying both sides with $e^{-i\lambda\alpha}$ and relabelling $|n\rangle e^{-i\lambda\alpha} \to |n\rangle$, to get

$$|n\rangle = |n^\circ\rangle + \sum_m{}' \frac{\langle m^\circ|\lambda \hat{H}'|n^\circ\rangle}{E_n^\circ - E_m^\circ} \underbrace{e^{-i\lambda\alpha}}_{1-\mathcal{O}(\lambda)} |m^\circ\rangle + \mathcal{O}(\lambda^2)$$

Keeping only terms up to order λ and setting $\lambda \to 1$ we finally have

$$\boxed{|n\rangle = |n^\circ\rangle + |n'\rangle = |n^\circ\rangle + \sum_m{}' \frac{\langle m^\circ|\hat{H}'|n^\circ\rangle}{E_n^\circ - E_m^\circ}|m^\circ\rangle}$$

$|n'\rangle$ is $\underbrace{\text{orthogonal to } |n^\circ\rangle}_{\text{i.e. } |n'\rangle = |n'_\perp\rangle}$ and linear in $\hat{H}'$.
— we eliminated $|n'_\parallel\rangle$ by normalizing and phase choice.

- To get the second order correction to E_n we collect from $(*)$ on p. 27 the terms $\sim \lambda^2$.

$$\boxed{\hat{H}^\circ|n^2\rangle + H'|n'\rangle = E_n^\circ|n^2\rangle + E_n'|n'\rangle + E_n^2|n^\circ\rangle}$$

and dot with $\langle n^\circ|$:

$$E_n^2 = \cancel{\langle n^\circ|\hat{H}^\circ|n^2\rangle} + \langle n^\circ|\hat{H}'|n'\rangle - \cancel{E_n^\circ\langle n^\circ|n^2\rangle} - E_n' \underbrace{\langle n^\circ|n'\rangle}_{0}$$

$$= \sum_m{}' \frac{\langle m^\circ|\hat{H}'|n^\circ\rangle}{E_n^\circ - E_m^\circ}\langle n^\circ|\hat{H}'|m^\circ\rangle$$

$$\boxed{= \sum_m{}' \frac{|\langle n^\circ|\hat{H}'|m^\circ\rangle|^2}{E_n - E_m^\circ}}$$

We stop here; the second order correction to the eigenstates is already quite messy.

General features:

- The energy at a given order involves knowledge of the state vector at one order lower only! (c.f. remarks when discussing the variational method)

- A necessary condition for the perturbation expansion to converge is that $\langle n' | n' \rangle \ll 1$,

i.e. $$\boxed{\left| \frac{\langle m^0 | \hat{H}' | n^0 \rangle}{E_n^0 - E_m^0} \right| \ll 1 \quad \forall\, n, m}$$

We see that if two states happen to have small energy difference $E_n^0 - E_m^0$ in the unperturbed case, this threatens the convergence of the perturbation series. If the two states are <u>degenerate</u>, $E_n^0 = E_m^0$, we have to proceed differently, using a method called <u>degenerate perturbation theory</u> to be discussed later in this chapter.