2

Time-Independent Perturbation Theory

2.1. Overview

2.1.1. General question

Assuming that we have a Hamiltonian,

\[ H = H^0 + \lambda H^1 \]  

(2.1)

where \( \lambda \) is a very small real number. The eigenstates of the Hamiltonian should not be very different from the eigenstates of \( H^0 \). If we already know all eigenstates of \( H^0 \), can we get eigenstates of \( H^1 \) approximately?

Bottom line: we are studying an approximate method.

2.1.2. Why perturbation theory?

Why we need to study this approximation methods? (considering the fact that numerical methods can compute the eigenstates very efficiently and accurately for any Hamiltonian that we consider in this course)

Reason number I: It is part of the history (QM was born before electronic computer becomes a powerful tool in scientific research).

Reason number II: It reveals to us universal principles, which are very important and cannot be obtained from just numerical simulations

Reason number III: The idea of perturbation theory has very deep and broad impact in many branches of physics. Perturbation theories is in many cases the only theoretical technique that we have to handle various complex systems (quantum and classical). Examples: in quantum field theory (which is in fact a nonlinear generalization of QM), most of the efforts is to develop new ways to do perturbation theory (Loop expansions, 1/N expansions, 4-\( \epsilon \) expansions).

2.1.3. Assumptions

Assumption #1: we know all eigenstates of \( H^0 \), as well as their corresponding eigenenergies

\[ H^0 \left| \psi_n^0 \right> = E_n^0 \left| \psi_n^0 \right> \]  

(2.2)

Assumption #2: we know the perturbation \( H^1 \). What do we mean by knowing \( H^1 \)? Here, we mean that we can write down \( H^1 \) using the complete basis of \( \left| \psi_n^0 \right> \), i.e., we know the value of \( \left< \psi_m^0 \mid H^1 \mid \psi_n^0 \right> \) for any \( m \) and \( n \).

Assumption #3: we only consider quantum states with discrete eigenenergies

In general, the energy spectrum of a quantum system (i.e. all eigenvalues of the Hamiltonian) falls into one of the following three general possibilities

- A discrete spectrum: eigenenergies can only take certain discredited values (example: infinite deep potential wells, e.g. harmonic potential \( E_n = (n + 1/2) \hbar \omega \))
A continuous spectrum: eigenenergies can take any (real) values in certain allowed range (example: a constant potential. Here, any \( E \geq V \) is an eigenenergy)

A mixed spectrum: some parts of the spectrum are continuous, while other parts have discrete eigenenergies. (example: a finite potential well. Here, we may have some discrete states inside the well. But for \( E \) above the top of the potential well, we have a continuous spectrum).

Q: Consider the energy spectrum of an attractive Coulomb \((1/r)\) potential. Is it discrete, continuous or mixed?

A: It is mixed. When we consider the an attractive Coulomb potential, we mostly focus on the negative energy states \((E < 0)\). This part of the spectrum is discrete, as we all know very well from the study of a hydrogen atom. But if we look at states with positive energies, there is a continuous spectrum for \( E > 0 \). For \( E > 0 \), the system is NOT a bound state, i.e. the proton and the electron doesn’t form an atom. In other words, we have a high probability found the proton and the electron to be separated far from each other. There, the attractive potential is very small and negligible, so we have two free particles and only need to consider their kinetic energies. For free particles, we know that any positive energy is an allowed eigenenergy (i.e. we have a continuum spectrum for \( E > 0 \)).

Bottom line: in this chapter, our perturbation theory only consider discrete spectrum or the discrete part of a mixed spectrum.

Another version of assumption #3: we only consider confined states. (In QM, in most cases, confined states=discrete energy and unconfined states=continuous energy).

Comment: In QM, we only study discrete states in a perturbation theory. But this is NOT true for other branches of physics. For example, in quantum field theory, perturbation theory is applied to continuous spectral.

### 2.2. Non-degenerate Perturbation Theory

#### 2.2.1. Assumptions

**Key assumption:** we consider a specific states \( \psi_n \). Here, we assume that \( E_n - E_m \) is much larger than \( \lambda H \) for any other eigenstate \( \psi_m \)

#### 2.2.2. Preparation #1 wavefunctions

Since the eigenstates of \( H_0 \) form a compete basis, we can write down any quantum state as a linear superposition of \( \psi_n \)

\[
|\psi\rangle = \sum_m a_m |\psi_m\rangle
\]  
(2.3)

Now, if we consider an eigenstate of \( H \), \( |\psi_n\rangle \), it can also be written in a similar fashion

\[
|\psi_n\rangle = \sum_m a_m |\psi_n\rangle
\]  
(2.4)

As discussion above, if \( \lambda \) is small, an eigenstate of \( H \) would be similar to an eigenstate of \( H_0 \). Here, we assume that \( |\psi_n\rangle \) is very close to \( |\psi_n^n\rangle \).

This means that \( a_n \approx 1 \) and for other values of \( m \neq n \), \( a_m \sim 0 \). To highlight this, we separate the term for \( |\psi_n^n\rangle \) out from the sum

\[
|\tilde{\psi}_n\rangle = a_n |\psi_n^n\rangle + \sum_{m \neq n} a_m |\psi_m^n\rangle
\]  
(2.5)

It turns out that it is usually more convenient to use unnormalized eigenstates. Now, let us define unnormalized eigenstates of \( H \)

\[
|\phi_n\rangle = \frac{1}{a_n} |\tilde{\psi}_n\rangle = |\phi_n^n\rangle + \sum_{m \neq n} a_m |\phi_m^n\rangle
\]  
(2.6)

For simplicity, we will now call \( a_n / a_m = c_m \)

\[
|\phi_n\rangle = |\phi_n^n\rangle + \sum_{m \neq n} c_m |\phi_m^n\rangle
\]  
(2.7)

Because \( a_m \sim 0 \) and \( a_n \sim 1 \), we know that \( c_m \sim 0 \) for small \( \lambda \).

**Comment #1:** This state is NOT normalized

\[
\langle \phi_n | \phi_n \rangle = 1 + \sum_{m \neq n} |c_m|^2 \geq 1
\]  
(2.8)