

Solving Perturbation Theory Problems

William Miyahira

Firstly, we need to identify the Hamiltonian for the problem and split it into two parts:

$$H = H_0 + \lambda V.$$

Here, H_0 is the Hamiltonian corresponding to a system that we know the exact eigenenergies and eigenstates:

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

where the superscript corresponds to the unperturbed energies and states. λV is the perturbation to the known Hamiltonian. The problem we want to solve is

$$(H_0 + \lambda V) |n\rangle = E_n |n\rangle.$$

Once we have the unperturbed states, we need to determine whether they are degenerate (multiple states have the same energy).

1 Non-Degenerate Perturbation Theory

If the eigenstates of H_0 are non-degenerate (each one has a unique energy), then we can use non-degenerate perturbation theory to find the corrections to the energy levels and eigenstates due to λV . We start by writing the state $|n\rangle$ and the energy shift $\Delta_n = E_n - E_n^{(0)}$ as

$$\begin{aligned} |n\rangle &= |n^{(0)}\rangle + \lambda |n^{(1)}\rangle + \lambda^2 |n^{(2)}\rangle \dots \\ \Delta_n &= \lambda \Delta_n^{(1)} + \lambda^2 \Delta_n^{(2)} + \dots \end{aligned}$$

where the superscripts correspond to the order of the perturbation. In general we will want to solve for the following:

1.1 Corrections to the Energy

- The first order correction to the energy shift is given by

$$\Delta_n^{(1)} = V_{nn} = \langle n^{(0)} | V | n^{(0)} \rangle = \int \psi_n^{(0)\star} V \psi_n^{(0)} d^3r.$$

- The second order correction to the energy shift is given by

$$\Delta_n^{(2)} = \sum_{k \neq n} \frac{|V_{nk}|^2}{E_n^{(0)} - E_k^{(0)}},$$

where

$$V_{nk} = \langle n^{(0)} | V | k^{(0)} \rangle.$$

1.2 Corrections to the State

The first order correction to the state is given by

$$|n^{(1)}\rangle = \sum_{k \neq n} \frac{V_{nk}}{E_n^{(0)} - E_k^{(0)}} |k^{(0)}\rangle.$$

2 Degenerate Perturbation Theory

If the eigenstates of H_0 are degenerate, then we need to solve the problem using degenerate perturbation theory.

1. First, find out which states are degenerate.
2. Consider a problem with m degenerate states. Construct the $m \times m$ perturbation matrix \mathbb{V} , whose elements are given by
$$\mathbb{V}_{ij} = \langle i^{(0)} | V | j^{(0)} \rangle.$$
3. Diagonalize the perturbation matrix. That is, find the eigenvalues and eigenstates of \mathbb{V} .
4. Once found, we see that
 - The eigenvalues of \mathbb{V} give the first order corrections to the energy shifts.
 - The eigenstates of \mathbb{V} give the correct zeroth-order kets that the perturbed kets approach in the limit $\lambda \rightarrow 0$ (no perturbation).

The main thing to note with the degenerate case is that when the perturbation is applied, the degeneracy is lifted. That is, the previously perturbed kets are put into the "correct" states, which are linear combinations of the unperturbed kets. The energies of these "correct" states are then shifted up or down from the degenerate energy, thus lifting the degeneracy of the system. However, sometimes not all the degeneracy is broken at first order, so sometimes the unperturbed kets are not affected by the perturbation (see the Linear Stark Effect in Sakurai page 319).

3 Time Dependent Problems

This section probably isn't necessary to know for the qualifying exam, but it's included just in case I suppose.

3.1 The Schrodinger Equation

The time-dependent Schrodinger equation is

$$H(t)\Psi(\mathbf{r}, t) = i\hbar \frac{\partial \Psi(\mathbf{r}, t)}{\partial t},$$

where $H(t) = H_0 + V(t)$. As before, H_0 is the "original" Hamiltonian for which we know the eigenenergies and eigenstates, E_n and $\phi_k(\mathbf{r})$. But this time, the perturbation depends on time. Since the eigenfunctions $\phi_k(\mathbf{r})$ form a complete set, we can write the solution to the time-dependent Schrodinger equation as

$$\Psi(\mathbf{r}, t) = \sum_k c_k(t) \phi_k(\mathbf{r}) e^{-i\omega_k t},$$

where $\omega_k = E_k/\hbar$. Plugging this into the Schrodinger equation yields

$$H(t)\Psi(\mathbf{r}, t) = (H_0 + V(t)) \sum_k c_k(t) \phi_k(\mathbf{r}) e^{-i\omega_k t} = i\hbar \left(\frac{\partial}{\partial t} \right) \sum_k c_k(t) \phi_k(\mathbf{r}) e^{-i\omega_k t}.$$

Now if we multiply from the left by $\phi_j(\mathbf{r})^*$ and integrate over \mathbf{r} , then we get

$$i\hbar \frac{dc_j(t)}{dt} = \sum_k c_k(t) V_{jk}(t) e^{i\omega_{jk} t},$$

where $V_{jk}(t) = \langle \phi_j | V(t) | \phi_k \rangle$ and $\omega_{jk} = \omega_j - \omega_k$. This gives us a system of coupled differential equations for the coefficients $c_j(t)$. By looking at the quantity $|c_j(t)|^2$, we can obtain the probability that the system will be found in the state j as a function of time.

3.2 The Interaction Picture

Using the interaction picture, the transition probability for going from state $|i\rangle \rightarrow |n\rangle$ with $n \neq i$ is given by

$$P(i \rightarrow n) = |c_n^{(1)}(t) + c_n^{(2)}(t) + \dots|^2,$$

with

$$\begin{aligned} c_n^{(0)}(t) &= \delta_{ni}, \\ c_n^{(1)}(t) &= -\frac{i}{\hbar} \int_{t_0}^t \langle n | V_I(t') | i \rangle dt' = -\frac{i}{\hbar} \int_{t_0}^t e^{i\omega_{ni} t'} V_{ni}(t') dt', \\ c_n^{(1)}(t) &= -\left(\frac{i}{\hbar}\right)^2 \sum_m \int_{t_0}^t dt' \int_{t_0}^{t'} dt'' e^{i\omega_{nm} t'} V_{nm}(t') e^{i\omega_{nm} t''} V_{mi}(t''). \end{aligned}$$

We have used

$$e^{i(E_n - E_m)t/\hbar} = e^{i\omega_{ni} t}.$$