11. Time Independent Perturbation Theory

Objective: determine the eigenfunctions and eigenvalues of a Hamiltonian

$\hat{H} = \hat{H}^0 + \lambda \hat{H}'$

where $\hat{H}^0$ is a known solution for a similar problem, and $\hat{H}'$ is the perturbation from this. The matrix elements of $\hat{H}^0$ and $\hat{H}'$ are of the same size.

λ is a small number, so if $\hat{H}^0$ and $\hat{H}'$ are the same size, the latter will give a small contribution to the result. λ is real, $|\lambda| << 1$.

We assume that we know the eigenfunctions and eigenvalues of $\hat{H}^0$,

$$\hat{H}^0 \varphi_n^0 = E_n^0 \varphi_n^0$$

with φ_n^0 orthonormal and E_n^0 non-degenerate.

We would like to solve

$$\hat{H}\varphi_n = E_n \varphi_n \quad (11\text{-}1)$$

As λ is a small number, we can expand around it.

$$\varphi_n = \varphi_n^0 + \lambda \varphi_n' + 0(\lambda^2)$$
$$E_n = E_n^0 + \lambda E_n' + 0(\lambda^2)$$

We chose the phase of φ_n such that

$$\langle \varphi_n, \varphi_n^0 \rangle = 0 \quad (11\text{-}2)$$

$$\left(\hat{H}^0 + \lambda \hat{H}'\right)\left(\varphi_n^0 + \lambda \varphi_n'\right) = \left(E_n^0 + \lambda E_n'\right)\left(\varphi_n^0 + \lambda \varphi_n'\right)$$

At order λ^0:

$$\hat{H}'\varphi_n^0 + \hat{H}^0 \varphi_n' = E_n^0 \varphi_n' + E_n' \varphi_n^0 \quad (11\text{-}3)$$

We take the scalar product with φ_n^0:

$$\langle \varphi_n^0, \hat{H}'\varphi_n^0 \rangle + \langle \varphi_n^0, \hat{H}^0 \varphi_n' \rangle = E_n^0 \underbrace{\langle \varphi_n^0, \varphi_n' \rangle}_{0} + E_n' \underbrace{\langle \phi_n^0, \varphi_n^0 \rangle}_{1} \quad (11\text{-}4)$$

$$\langle \varphi_n^0, \hat{H}^0 \varphi_n' \rangle = \left\langle \underbrace{\hat{H}^0 \varphi_n^0}_{E_n^0 \varphi_n^0}, \varphi_n' \right\rangle = E_n^0 \underbrace{\langle \varphi_n^0, \varphi_n' \rangle}_{0}$$

$$E_n' = \langle \varphi_n^0, \hat{H}'\varphi_n^0 \rangle$$

So we can say that the total energy is

$$E_n = E_n^0 + \lambda E_n'$$
$$= E_n^0 + \lambda \langle \varphi_n^0, \hat{H}', \varphi_n^0 \rangle$$

Going back to (11-3), and taking the scalar product with φ_i^0 $(i \neq n)$:

$$\langle \varphi_i^0, \hat{H}', \varphi_n^0 \rangle + \langle \varphi_i^0, \hat{H}^0, \varphi_n' \rangle = E_n^0 \langle \varphi_i^0, \varphi_n' \rangle + E_n' \langle \varphi_i^0, \varphi_n^0 \rangle \quad (11\text{-}6)$$

We know that $\langle \varphi_i^0, \varphi_n^0 \rangle = 0$, and $\langle \varphi_i^0, \hat{H}^0, \varphi_n' \rangle = \langle \hat{H}^0 \varphi_i^0, \varphi_n' \rangle = E_i^0 \langle \varphi_i^0, \varphi_n' \rangle$. So, (11-6) can be written as:

$$\langle \varphi_i^0, \hat{H}', \varphi_n^0 \rangle = E_n^0 \langle \varphi_i^0, \varphi_n' \rangle - E_i \langle \varphi_i^0, \varphi_n' \rangle$$

$$\langle \varphi_i^0, \varphi_n' \rangle = \frac{\langle \varphi_i^0, \hat{H}', \varphi_n^0 \rangle}{E_n^0 - E_i^0} \quad (11\text{-}7)$$

φ_n' is an orthonormal basis of the state space. We can write any eigenfunction as a linear combination:

$$\varphi_{n'} = \sum_p c_p \varphi_p^0 ,$$

where

$$c_p = \langle \varphi_p^0, \varphi_n' \rangle .$$

We know that $\langle \varphi_n^0, \varphi_n' \rangle = 0$, hence $c_n = 0$. So we can write

$$\varphi_{n'} = \sum_{p \neq n} c_p \varphi_p^0$$

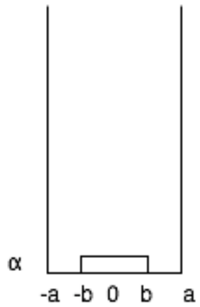
Using the equation for $\langle \varphi_i^0, \varphi_n' \rangle$ above, we can write:

$$\varphi_{n'} = \sum_{p \neq n} \frac{\langle \varphi_p^0, \hat{H}', \varphi_n^0 \rangle}{E_n^0 - E_p^0} \varphi_p^0$$

So we can write

$$\varphi_n = \varphi_n^0 + \lambda \varphi_n'$$

Example: find the eigenfunctions and eigenvalues to the first order α of the Hamiltonian corresponding to the potential



$\hat{H}^0 =$ infinite square well. $|\alpha| << 1$

$$\hat{H} = \hat{H}^0 + \alpha \hat{H}'$$

$$\hat{H}' = \begin{cases} 1 & |x| \leq b \\ 0 & |x| > b \end{cases}$$

We know that the energy for an infinite square well is:

$$E_n^0 = \frac{n^2 \pi^2 \hbar^2}{8a^2 m}$$

$$\varphi_n^0 = \begin{cases} \frac{1}{\sqrt{a}} \cos \frac{n\pi x}{2a} & n \text{ odd} \\ \frac{1}{\sqrt{a}} \sin \frac{n\pi x}{2a} & n \text{ even} \end{cases}$$

We said before that

$$E_n' = \langle \varphi_n^0, \hat{H}' \varphi_n^0 \rangle$$

Let's look at the correction to the energy level, with $n=1$, and using $\varphi_1{}^0 = \frac{1}{\sqrt{a}}\cos\frac{nx}{2a}$, we can write:

$$E_1' = \left\langle \varphi_1{}^0, \hat{H}'\varphi_1{}^0 \right\rangle = \frac{1}{a}\int_{-b}^{b} \cos\frac{nx}{2a} 1 \frac{\cos nx}{2a} dx = \frac{b}{a} + \frac{1}{\pi}\sin\frac{\pi b}{a}$$

So the first energy level is:

$$E_1 = \frac{\pi^2\hbar^2}{8a^2m} + \alpha\left(\frac{b}{a} + \frac{1}{\pi}\sin\left(\frac{\pi b}{a}\right)\right)$$

Now look at the second energy level.

$$E_2' = \left\langle \varphi_2{}^0, \hat{H}'\varphi_2{}^0 \right\rangle = \frac{1}{a}\int_{-b}^{b} \sin\frac{\pi x}{a}\sin\frac{\pi x}{a} dx = \frac{b}{a} - \frac{1}{2\pi}\sin\frac{2\pi b}{a}$$

So the second energy level is:

$$E_2 = \frac{4\pi^2\hbar^2}{8a^2m} + \alpha\left[\frac{b}{a} - \frac{1}{2\pi}\sin\frac{2\pi b}{a}\right]$$

Now look at $\left\langle \varphi_p{}^0, \hat{H}'\varphi_n{}^0 \right\rangle$. $p \neq n$.

$$\left\langle \varphi_p{}^0, \hat{H}'\varphi_n{}^0 \right\rangle = \int_{-b}^{b} \varphi_p{}^0 \varphi_n{}^0 dx$$

If n is odd, then φ_n will be even. If p is even, then φ_p in odd.
The scalar product will be 0 if p and n are of different parity (i.e. one odd, one even). It will be none-zero if p and n are either both even, or both odd.

So, if n is odd, p will have to be odd, and $\varphi_n{}'$ (from (11-7)) is a linear combination of even functions, so it is even. The same applies for odd functions.