Perturbation Theory Notes

Write

$$H = H_0 + \lambda V \tag{1}$$

Here H represents the problem of interest when $\lambda = 1$. H_0 represents a problem with known solutions. We can think about *turning on* the perturbation from $\lambda = 0$.

Let us take H_0 to be the particle in a box problem, and take the perturbation, V as

$$V(x) = ax - \frac{aL}{2} \tag{2}$$

so that the perturbation is symmetrical and shouldn't raise the overall energy of the particle.

For the particle in a box we have

$$H_0 \phi_n^{(0)} = E_n^{(0)} \phi_n^{(0)} \tag{3}$$

with

$$E_n^{(0)} = \frac{n^2 \pi^2 \hbar^2}{2mL^2} \tag{4}$$

and

$$\phi_n^{(0)} = \sqrt{2/L} \sin(n\pi x/L) \tag{5}$$

Recall that the set $\{\phi_n^{(0)}\}$ forms a *basis*, where $n \in [1, \infty)$.

Let ϕ_n, E_n be the fully perturbed ($\lambda = 1$) wavefunctions and energies, $H\phi_n = E_n\phi_n$.

We seek a perturbative expansion (a power series) of the form

$$E_n = E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots \tag{6}$$

$$\phi_n = \phi_n^{(0)} + \lambda \phi_n^{(1)} + \lambda^2 \phi_n^{(2)} + \cdots \tag{7}$$

Substituting into $H\phi_n = E_n\phi_n$ yields

$$\begin{aligned} (H_0 + \lambda V)\left(\phi_n^{(0)} + \lambda \phi_n^{(1)} + \lambda^2 \phi_n^{(2)} + \cdots\right) = \\ \left(E_n^{(0)} + \lambda E_n^{(1)} + \lambda^2 E_n^{(2)} + \cdots\right)\left(\phi_n^{(0)} + \lambda \phi_n^{(1)} + \lambda^2 \phi_n^{(2)} + \cdots\right) \end{aligned} \tag{8}$$

To proceed we equate like powers of λ. This is because we want this expression to hold for any value of λ. The easiest way to see that we should collect powers of λ is to set $\lambda = 0$, which gives us the expression containing only *zeroth* powers. Next, we take $d/d\lambda$ on both sides and evaluate at $\lambda = 0$, which gives us the expression containing only *first* powers. Next, we take $d^2/d\lambda^2$ on both sides and evaluate at $\lambda = 0$, which gives us the expression containing only *second* powers. And so on. Let us write down these expressions.

$$\lambda^0 : \qquad H_0\phi_n^{(0)} = E_n^{(0)}\phi_n^{(0)} \tag{9}$$

$$\lambda^1 : \qquad H_0\phi_n^{(1)} + V\phi_n^{(0)} = E_n^{(0)}\phi_n^{(1)} + E_n^{(1)}\phi_n^{(0)} \tag{10}$$

The zeroth power expression is just the unperturbed problem. To proceed with the first power expression we expand $\phi_n^{(1)}$ using our basis set $\{\phi_n^{(0)}\}$

$$\phi_n^{(1)} = \sum_{\ell=1}^{\infty} c_\ell \phi_\ell^{(0)} \tag{11}$$

This gives

$$H_0 \sum_{\ell=1}^{\infty} c_\ell \phi_\ell^{(0)} + V\phi_n^{(0)} = E_n^{(0)} \sum_{\ell=1}^{\infty} c_\ell \phi_\ell^{(0)} + E_n^{(1)}\phi_n^{(0)} \tag{12}$$

In the expression we known that

$$H_0 \sum_{\ell=1}^{\infty} c_\ell \phi_\ell^{(0)} = \sum_{\ell=1}^{\infty} c_\ell E_\ell^{(0)} \phi_\ell^{(0)} \tag{13}$$

Making this replacement, we now multiply on both sides by $\phi_s^{(0)}$ and integrate

$$\sum_{\ell=1}^{\infty} c_\ell E_\ell^{(0)} \delta_{s\ell} + \int_0^L V(x)\phi_s^{(0)}\phi_n^{(0)}\,dx = E_n^{(0)} \sum_{\ell=1}^{\infty} c_\ell \delta_{s\ell} + E_n^{(1)}\delta_{sn} \tag{14}$$

Defining (this is matrix element notation)

$$\int_0^L V(x)\phi_s^{(0)}\phi_n^{(0)}\,dx = V_{sn} \tag{15}$$

we have, after collapsing the sums,

$$c_s E_s^{(0)} + V_{sn} = c_s E_n^{(0)} + E_n^{(1)}\delta_{sn} \tag{16}$$

For $s = n$ we have

$$E_n^{(1)} = V_{nn} \tag{17}$$

For $s \neq n$ we have

$$c_s E_s^{(0)} + V_{sn} = c_s E_n^{(0)} \tag{18}$$

which yields (non-degenerate case)

$$c_s = \frac{V_{sn}}{E_n^{(0)} - E_s^{(0)}} \tag{19}$$

Thus, to first order, we have

$$E_n = E_n^{(0)} + \lambda V_{nn} + \cdots \tag{20}$$

$$\phi_n = \phi_n^{(0)} + \lambda \sum_{\ell \neq n} \frac{V_{\ell n}}{E_n^{(0)} - E_\ell^{(0)}}\phi_\ell^{(0)} + \cdots \tag{21}$$