Time Independent Perturbation Theory

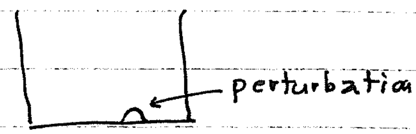
Suppose we know the solutions ψ_n to a known potential energy:

$$H^0 \psi_n^0 = E_n^0 \psi_n^0 \qquad \Rightarrow \text{ complete orthonormal set of w.f.s}$$

$$\langle \psi_n^0 | \psi_m^0 \rangle = \delta_{n,m}$$

with corresponding energies E_n^0

Perturb the potential slightly



<u>Perturbation theory</u> is a systematic procedure for obtaining approximate solutions to the perturbed problem, by building on the known exact solutions to the unperturbed case.

$$H = H^0 + \lambda H' \qquad \text{take } \lambda \text{ to be small, then } \lambda \to 1$$

$$\psi_n = \psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \cdots$$

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

$$H\psi_n \to (H^0 + \lambda H')(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \cdots)$$

$$= (E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots)(\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \cdots)$$

Collecting like powers of λ, we obtain

$$H\psi_n = E_n^0 \psi_n^0 + \lambda(E_n^1 \psi_n^0 + E_n^0 \psi_n^1) + \lambda^2(E_n^2 \psi_n^0 + E_n^1 \psi_n^1 + E_n^0 \psi_n^2) + \cdots$$

Lowest Order $\Rightarrow$ $H^0 \psi_n^0 = E_n^0 \psi_n^0$ "nothing new"

To 1st order λ $\Rightarrow$ $H'\psi_n^0 + H^0\psi_n^1 = E_n^1\psi_n^0 + E_n^0\psi_n^1$ (1)

To 2nd order in λ $\Rightarrow$ $H'\psi_n^1 + H^0\psi_n^2 = E_n^2\psi_n^0 + E_n^1\psi_n^1 + E_n^0\psi_n^2$ (2)

We're finished with λ. So, set $\lambda \to 1$.

FIRST ORDER PETURBATION THEORY

Take the "inner product" of (1) with $\langle\psi_n^0| = \psi_n^{0*}$

$$\langle\psi_n^0|H'|\psi_n^0\rangle + \langle\psi_n^0|H^0|\psi_n^1\rangle = E_n^1 \underbrace{\langle\psi_n^0|\psi_n^0\rangle}_{=1} + E_n^0 \underbrace{\langle\psi_n^0|\psi_n^1\rangle}$$

But H^0 is hermitian, so, in the 2nd term on the left

$$\langle\psi_n^0|H^0|\psi_n^1\rangle = \langle H^0\psi_n^0|\psi_n^1\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle$$

So, now we have: $\boxed{\langle\psi_n^0|H'|\psi_n^0\rangle = E_n^1}$ FIRST ORDER PERTURBATION THEORY

$\Rightarrow$ Example 6.1 in the book

FIND THE 1st ORDER CORRECTION TO THE WAVE FUNCTION

Starting with (1) up above

$$(H^0 - E_n^0)\psi_n^1 = -(H' - E_n^1)\psi_n^0 \qquad (3)$$

We know the right side, so, the above equation is an inhomogeneous differential equation in ψ_n^1.

We can express the ψ_n' wave functions in terms of a power series whose basis functions are the zeroth order wave functions

$$\psi_n' = \sum_{m \neq n} c_m^{(n)} \psi_m^\circ \qquad (4)$$

Substituting Eq. 4 into Eq. 3, we have

$$\left(H^\circ - E_n^\circ\right) \sum_{m \neq n} c_m^{(n)} \psi_m^\circ = -\left(H' - E_n'\right)\psi_n^\circ$$

$$\sum_{m \neq n} \left(E_m^\circ - E_n^\circ\right) c_m^{(n)} \psi_m^\circ = -\left(H' - E_n'\right)\psi_n^\circ$$

$\langle \psi_\ell^\circ |$ Take the inner product of both sides.

$$\sum_{m \neq n} \left(E_m^\circ - E_n^\circ\right) c_m^{(n)} \underbrace{\langle \psi_\ell^\circ | \psi_m^\circ \rangle}_{\delta_{\ell m}} = -\langle \psi_\ell^\circ | H' | \psi_n^\circ \rangle + E_n' \overbrace{\underbrace{\langle \psi_\ell^\circ | \psi_n^\circ \rangle}_{\delta_{\ell n}}}^{=0 \text{ for } \ell = n}$$

$$\left(E_\ell^\circ - E_n^\circ\right) c_\ell^{(n)} = -\langle \psi_\ell^\circ | H' | \psi_n^\circ \rangle \quad \text{for } \ell \neq n$$

(non-zero)

$\ell \to m$ to keep notation consistent with the normal way of writing this.

$$\left(E_m^\circ - E_n^\circ\right) c_m^{(n)} = -\langle \psi_m^\circ | H' | \psi_n^\circ \rangle$$

$$c_m^{(n)} = \frac{\langle \psi_m^\circ | H' | \psi_n^\circ \rangle}{E_n^{(0)} - E_m^{(0)}}$$

Eq. 4 $\Rightarrow$

$$\boxed{\psi_n' = \sum_{m \neq n} \frac{\langle \psi_m^\circ | H' | \psi_n^\circ \rangle}{E_n^\circ - E_m^\circ} \psi_m^\circ}$$

Problem 6.1 A δ-function bump in the center of an infinite well.

$$H' = \alpha\,\delta(x - a/2) \qquad \text{where} \quad \alpha = \text{constant} \quad (\text{Energy})$$

a.) Find the 1st order correction to the allowed energies.

$$\psi_n^0 = \sqrt{\frac{2}{a}}\,\sin\frac{n\pi x}{a} \qquad E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle = \frac{2}{a}\,\alpha\int_0^a \sin^2\frac{n\pi x}{a}\,\delta\left(x-\frac{a}{2}\right)dx$$

$$E_n^1 = \frac{2}{a}\,\alpha\,\sin^2\frac{n\pi}{2} = \begin{cases} 0 & \text{for } n = \text{even} \\ \frac{2\alpha}{a} & \text{for } n = \text{odd} \end{cases}$$

The even "n" wavefunctions don't feel the perturbation, H'.

b.) Find the first three non-zero terms in the expansion of ψ_n^1 ← 1st order correction.
of the correction to the ground state → ψ_1^1 ← n=1

$$\psi_1^1 = \sum_{m\neq 1}\frac{\langle\psi_m^0|H'|\psi_1^0\rangle}{E_1^0 - E_m^0}\,\psi_m^0$$

Let's look at $\langle\psi_m^0|H'|\psi_1^0\rangle = \frac{2\alpha}{a}\int_0^a \sin\frac{m\pi x}{a}\,\delta\left(x-\frac{a}{2}\right)\sin\frac{\pi x}{a}\,dx$

$$= \frac{2\alpha}{a}\,\sin\frac{m\pi}{2}\,\sin\frac{\pi}{2} = \frac{2\alpha}{a}\,\sin\left(\frac{m\pi}{2}\right)$$

$$\langle\psi_m^0|H'|\psi_1^0\rangle = \begin{cases} 0 & \text{for } m = \text{even} \\ \frac{2\alpha}{a}\,\sin\frac{m\pi}{2} & \text{for } m = 3, 5, 7, 9, \ldots \end{cases}$$

Problem 6.1 continued

Let's look at the denominator: $E_1^0 - E_m^0 = \frac{\pi^2\hbar^2}{2ma^2}(1-m^2)$

So, ψ_1' becomes:

$$\psi_1' = \sum_{m=3,5,7,\ldots} \frac{\frac{2\alpha}{a}\sin\frac{m\pi}{2}}{E_1^0 - E_m^0}\psi_m^0 = \frac{2\alpha}{a}\frac{2ma^2}{\pi^2\hbar^2}\left[\frac{-1}{1-9}\psi_3^0 + \frac{1}{1-25}\psi_5^0 - \frac{1}{1-49}\psi_7^0 + \cdots\right]$$

$$\psi_1' = \frac{4m\alpha a}{\pi^2\hbar^2}\sqrt{\frac{2}{a}}\left[\frac{1}{8}\sin\frac{3\pi x}{a} - \frac{1}{24}\sin\frac{5\pi x}{a} + \frac{1}{48}\sin\frac{7\pi x}{a} + \cdots\right]$$

$$\psi_1' = \frac{m\alpha}{\pi^2\hbar^2}\sqrt{\frac{a}{2}}\left[\sin\frac{3\pi x}{a} - \frac{1}{3}\sin\frac{5\pi x}{a} + \frac{1}{6}\sin\frac{7\pi x}{a} + \cdots\right]$$