11/30/98

Lecture #36 Perturbation Theory

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

Unperturbed

$$H^0 \psi_n^0 = E_n^0 \psi_n^0$$

assume both E_n^0 and ψ_n^0 are known

$$\langle \psi_n^0 | \psi_m^0 \rangle = \delta_{nm}$$

Like to solve $\quad H \psi_n = E_n \psi_n$

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

Method works best if $\lambda H'$ is small. λ is a device for counting powers of small perturbation H' at end interested in $\lambda = \underline{1}$.

Example $\quad \frac{p^2}{2m} \Rightarrow -\frac{\hbar^2}{2m} \frac{d^2}{dx^2}$

nonrel. kinetic energy.

Should have used $\sqrt{p^2 c^2 + m^2 c^4} - mc^2$

$$\simeq \frac{p^2}{2m} - \frac{p^4}{8m^3c^2}$$

Thus a relativistic correction to the nonrel. Hamiltonian is

$$H' = -\frac{p^4}{8m^3c^2} = -\frac{\hbar^4}{8m^3c^2}\frac{\partial^4}{\partial x^4}$$

In general this is a very small correction because $p \ll mc$ ie $v/c \ll 1$

$$H^0 = \frac{p^2}{2m} + V, \qquad H' = -\frac{p^4}{8m^3c^2}$$

But pert. theory works for lots of problems

Expand wave function and eigenvalue in power series in λ

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

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

$$\left[H^0 + \lambda H'\right]\left[\psi_n^0 + \lambda \psi_n^1 + \lambda^2 \psi_n^2 + \ldots\right] =$$

$$\left[E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \ldots\right]\left[\psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \ldots\right]$$

equate powers of λ (and set $\lambda = 1$)

λ^0: $H^0\psi_n^0 = E_n^0\psi_n^0$ unpert. problem.

$$\lambda^1: \quad H^0\psi_n^1 + \cancel{\lambda} H'\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0 \qquad \text{A}$$

$$\lambda^2: \quad H^0\psi_n^2 + H'\psi_n^1 = E_n^0\psi_n^2 + E_n^1\psi_n^1 + E_n^2\psi_n^0 \qquad \text{B}$$

Take innerproduct of A with ψ_n^0 and set $\lambda = 1$

$$\langle\psi_n^0|H^0|\psi_n^1\rangle + \langle\psi_n^0|H'|\psi_n^0\rangle$$

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

$\langle\psi_n^0 H^0\psi_n^1\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle$ let H^0 act to left.

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

$$\boxed{E_n^1 = \langle\psi_n^0|H'|\psi_n^0\rangle}$$

1st order shift in energy. This is just expectation of perturbation in unperturbed wave function.

To find 1st order correction to wave function 3 rewrite Ⓐ

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

Expand $\psi_n^1 = \sum_{n \neq m} c_m^{(n)} \psi_m^0$

In general pert. will mix in a little bit of all of the other states $m \neq n$ into ψ_n^0.

$$\sum_{m \neq n} (H^0 - E_n^0) c_m^n \psi_m^0 = -(H' - E_n^1)\psi_n^0$$

Take inner product with ψ_l^0

$$\sum_{m \neq n} (E_m^0 - E_n^0) c_m^n \langle \psi_l^0 | \psi_m^0 \rangle = -\langle \psi_l^0 | H' | \psi_n^0 \rangle + E_n^1 \langle \psi_l^0 | \psi_n^0 \rangle$$

assume $l \neq n$ then $\langle \psi_l^0 | \psi_m^0 \rangle = \delta_{lm}$

$$(E_l^0 - E_n^0)\, c_l^n = -\langle \psi_l^0 | H' | \psi_n^0 \rangle$$

or

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

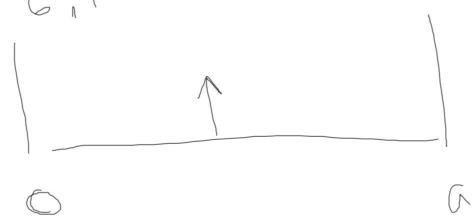
$$\boxed{\psi_n^1 = \sum_{m \neq n} \frac{\langle \psi_m^0 | H' | \psi_n^0 \rangle}{E_n^0 - E_m^0} \psi_m^0}$$

Note normalization $\langle \psi_n^1 | \psi_n^0 \rangle = 0$

So total wave function $\langle \psi_n^0 + \psi_n^1 | \psi_n^0 \rangle = 1$
Possible problem if energy eigenvalues are degenerate. Then denominator can vanish. Assume unpert. spectrum is nondegenerate for now. Then $m \neq n$ in sum is enough to keep energy from vanishing.
denom.

Example problem 6.1

Square well with δ func.



$$H' = \alpha\, \delta(x - a/2)$$ assume α small

Need unp. wave functions and energies

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

$$\psi_n^0(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a} x\right)$$

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

$$= \int_0^a dx\, \frac{2}{a} \sin^2\left(\frac{n\pi}{a} x\right) \alpha\, \delta(x - a/2)$$

$$= \frac{2}{a} \alpha \sin^2\left(n \frac{\pi}{2}\right) = \begin{cases} \frac{2}{a}\alpha & n \text{ odd} \\ 0 & n \text{ even} \end{cases}$$