Perturbation theory

Read McIntyre 10.3-10.4

PH451/551

Recap – matrix representation of operators

Operators can be represented symbolically
(x, p, H, a)

Operators can be represented as functions and derviatives
(x, (h/i)d/dx, ….

Operators can be represented as matrices
(basis usually that of the eigenfunctions of H)

Matrix representation of operators

$$\hat{Q} = \begin{pmatrix} Q_{00} & Q_{01} & Q_{03} & \cdots \\ Q_{10} & Q_{11} & Q_{12} & \cdots \\ Q_{20} & Q_{21} & Q_{22} & \cdots \\ \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$$\begin{array}{c} \\ \langle 0| \\ \langle 1| \\ \langle 2| \\ \langle 3| \end{array} \begin{array}{cccc} |0\rangle & |1\rangle & |2\rangle & |3\rangle \\ \end{array}$$

$$\begin{pmatrix} Q_{00} & Q_{01} & Q_{02} & \cdots \\ Q_{10} & Q_{11} & Q_{12} & \cdots \\ Q_{20} & Q_{21} & Q_{22} & \cdots \\ \vdots & \vdots & \vdots & \end{pmatrix}$$

$$Q_{mn} = \langle m|\hat{Q}|n\rangle$$

$$= \int_{-\infty}^{\infty} \varphi_m(x)\hat{Q}\varphi_n(x)\,dx$$

Reading Quiz

In the expression $H = H_0 + \lambda H'$

1. What does H_0 represent?

2. What does H' represent?

3. What does λ represent?

Reading Quiz

In the expression $H = H_0 + \lambda H'$

1. What does H_0 represent?
   The "original Hamiltonian" of some system whose solution is known.
2. What does H' represent?
   The "perturbation Hamiltonian" – a small term relative to H_0 .
3. What does λ represent?
   It is a bookkeeping device that keeps track of the order of the small quantities.

Main results (energy)

1. The 0th order energy of the *n*th eigenstate (or "unperturbed energy") – assumed known

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)}$$

2. The first order correction to the energy of the *n*th eigenstate.

$$E_n^{(1)} = \left\langle n^{(0)} \middle| H' \middle| n^{(0)} \right\rangle$$

3. 2nd:

$$E_n^{(2)} = \sum_{m \neq n} \frac{\left| \left\langle m^{(0)} \middle| H' \middle| n^{(0)} \right\rangle \right|^2}{\left(E_n^{(0)} - E_m^{(0)} \right)}$$

Main results (state)

1. The 0th order *n*th eigenstate (or "unperturbed state") – assumed known

$$\left|n\right\rangle = \left|n^{(0)}\right\rangle + \left|n^{(1)}\right\rangle$$

2. The first order correction to the *n*th eigenstate.

$$\left|n\right\rangle = \left|n^{(0)}\right\rangle + \sum_{m \neq n} \frac{\left\langle m^{(0)} \right| H' \left| n^{(0)} \right\rangle}{\left(E_n^{(0)} - E_m^{(0)}\right)} \left|m^{(0)}\right\rangle$$

Example HO

1. Add *E* field to 1-D HO Hamiltonian
2. *H'*=? Now calculate first order correction to energy

$$E_n^{(1)} = \left\langle n^{(0)} \middle| H' \middle| n^{(0)} \right\rangle$$

Example - HO

1. Add *E* field to 1-D HO Hamiltonian
2. Now calculate first order correction to state

$$\left|n^{(1)}\right\rangle = \sum_{m\neq n} \frac{\left\langle m^{(0)}\right| H' \left|n^{(0)}\right\rangle}{\left(E_n^{(0)} - E_m^{(0)}\right)} \left|m^{(0)}\right\rangle$$

Set up – and power series approach

1. Full eignvalue equation

$$H|n\rangle = E_n|n\rangle$$

2. Hamiltonian = original plus change

$$\left(H_0 + H'\right)|n\rangle = E_n|n\rangle$$

3. Assume series approach is valid

$$E_n = E_n^{(0)} + E_n^{(1)} + E_n^{(2)} + \ldots$$

$$|n\rangle = \left|n^{(0)}\right\rangle + \left|n^{(1)}\right\rangle + \left|n^{(2)}\right\rangle \ldots$$

Plug in ….

$$H\left|n\right\rangle = E_n\left|n\right\rangle$$

$$\left(H_0 + H'\right)\left(\left|n^{(0)}\right\rangle + \left|n^{(1)}\right\rangle + \left|n^{(2)}\right\rangle \ldots\right)$$

$$= \left(E_n^{(0)} + E_n^{(1)} + E_n^{(2)} ..\right)\left(\left|n^{(0)}\right\rangle + \left|n^{(1)}\right\rangle + \left|n^{(2)}\right\rangle ..\right)$$

Plug in ....

$$H_0\left|n^{(0)}\right\rangle + H'\left|n^{(0)}\right\rangle + H_0\left|n^{(1)}\right\rangle$$

$$+H'\left|n^{(1)}\right\rangle + H_0\left|n^{(2)}\right\rangle \ldots$$

$$=$$

$$E_n^{(0)}\left|n^{(0)}\right\rangle + E_n^{(1)}\left|n^{(0)}\right\rangle + E_n^{(2)}\left|n^{(0)}\right\rangle$$

$$+E_n^{(0)}\left|n^{(1)}\right\rangle + E_n^{(1)}\left|n^{(1)}\right\rangle + E_n^{(0)}\left|n^{(2)}\right\rangle \ldots$$

Derivation – 1st order energy

1. First order equation

$$\left(H_0 - E_n^{(0)}\right)\left|n^{(1)}\right\rangle = \left(E_n^{(1)} - H'\right)\left|n^{(0)}\right\rangle$$

$$\left\langle n^{(0)}\right|\left(H_0 - E_n^{(0)}\right)\left|n^{(1)}\right\rangle = \left\langle n^{(0)}\right|\left(E_n^{(1)} - H'\right)\left|n^{(0)}\right\rangle$$

$$\left\langle n^{(0)}\right|\left(E_n^{(0)} - E_n^{(0)}\right)\left|n^{(1)}\right\rangle = E_n^{(1)} - \left\langle n^{(0)}\right|H'\left|n^{(0)}\right\rangle$$

$$E_n^{(1)} = \left\langle n^{(0)}\right|H'\left|n^{(0)}\right\rangle$$

$$E_n^{(1)} = H'_{nn}$$

"Hermitian operator can act backwards"

1. If

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

2. Then always true that

$$\left\langle n^{(0)} \right| H_0^{\dagger} = \left\langle n^{(0)} \right| E_n^{(0)*}$$

3. And for Hermitian operator

$$\left\langle n^{(0)} \right| H_0 = \left\langle n^{(0)} \right| E_n^{(0)}$$

Digression (1)
operator algebra - Hermitian

1. Hermitian conjugate is defined as the complex conjugate of the transpose in matrix language.

$$H^{\dagger}{}_{ij} \equiv H_{ji}{}^{*} (Hermitian\ conj)$$

$$\langle i | H^{\dagger} | j \rangle \equiv \langle j | H | i \rangle^{*} = \langle j | Hi \rangle^{*} = \langle Hi | j \rangle$$

$$\langle i | H^{\dagger} \equiv \langle Hi |$$

2. This is what is meant by “acting backwards” – act on the bra with the Hermitian conjugate

$$\langle i | H \equiv \langle H^{\dagger} i |$$

Digression (2)
operator algebra - Hermitian

3. Operator is "Hermitian" if it is equal to its Hermitian conjugate. That means if *H* is Hermitian

$$\langle i | H = \langle H i |$$

4. Hermitian operators are nice – the same operator can "act backwards and forwards"!

Derivation – 1st order state

1. First order equation: $\neq n$

$$\left(H_0 - E_n^{(0)}\right)\left|n^{(1)}\right\rangle = \left(E_n^{(1)} - H'\right)\left|n^{(0)}\right\rangle$$

$$\left\langle m^{(0)}\right|\left(H_0 - E_n^{(0)}\right)\left|n^{(1)}\right\rangle = \left\langle m^{(0)}\right|\left(E_n^{(1)} - H'\right)\left|n^{(0)}\right\rangle$$

$$\left\langle m^{(0)}\right|\left(E_m^{(0)} - E_n^{(0)}\right)\left|n^{(1)}\right\rangle = -\left\langle m^{(0)}\right|H'\left|n^{(0)}\right\rangle$$

assume $$\left|n^{(1)}\right\rangle = \sum_{p\neq n} c_{np}\left|p^{(0)}\right\rangle$$

Derivation – 1st order state

$$\left|n^{(1)}\right\rangle = \sum_{p \neq n} c_{np}\left|p^{(0)}\right\rangle$$

This says: I can write the "correction" to the nth state as a superposition of unperturbed states. Finding the correction is equivalent to finding the c_{np} values (I know the unperturbed states).

Derivation – 1st order state

1. First order equation

$$\langle m^{(0)}|\left(E_m^{(0)}-E_n^{(0)}\right)|n^{(1)}\rangle=-\langle m^{(0)}|H'|n^{(0)}\rangle$$

assume $$|n^{(1)}\rangle=\sum_{p\neq n}c_{np}|p^{(0)}\rangle$$

$$\langle m^{(0)}|\left(E_m^{(0)}-E_n^{(0)}\right)\sum_{p\neq n}c_{np}|p^{(0)}\rangle=-H'_{mn}$$

$$\sum_{p\neq n}c_{np}\langle m^{(0)}|1|p^{(0)}\rangle\left(E_m^{(0)}-E_n^{(0)}\right)=-H'_{mn}$$

Derivation – 1st order state

1. First order equation

$$\sum_{p \neq n} c_{np} \left(E_m^{(0)} - E_n^{(0)} \right) \langle m^{(0)} | 1 | p^{(0)} \rangle = -H'_{mn}$$

$$\sum_{p \neq n} c_{np} \delta_{mp} \left(E_m^{(0)} - E_n^{(0)} \right) = -H'_{mn}$$

$$c_{nm} = \frac{H'_{mn}}{\left(E_n^{(0)} - E_m^{(0)} \right)}$$

Derivation – 1st order state

1. First order correction is superposition of unpert. states:

$$\left|n^{(1)}\right\rangle = \sum_{m\neq n} c_{nm}\left|m^{(0)}\right\rangle$$

2. Coeffs:

$$\left|n^{(1)}\right\rangle = \sum_{m\neq n} \frac{H'_{mn}}{\left(E_n^{(0)} - E_m^{(0)}\right)}\left|m^{(0)}\right\rangle$$

Energy difference in denominator: “close states mix in more” (unless matrix element is zero!)

More examples

1. Perturb the HO to a slightly different frequency at $x>0$! (What weird spring is that?!)

2. Identify H'
3. First order energy
4. First order state
5. Second order energy

Things to note

1. When there is an off-diagonal term in the perturbation Hamiltonian, there are first order corrections to the wave function.
2. Nearby (in energy) states "mix in" to a larger degree than far-away ones
3. Degeneracy presents problems in this formulation – denominator blows up (need new strategy)
4. "Small" means that off-diagonal matrix element is small relative to energy separations
5. First order state is still normalized (see text)
6. One can, in principle, solve the eigenvalue equation numerically (diagonalize huge matrix or solve tricky diff. equation) to get an "exact" solution. BUT .....