Spring 1997 #10 (p 1 of 3)

Consider a Schrödinger eigenvalue problem of the form

$$H|i\rangle = E_i|i\rangle \quad , i = 1,2,\dots$$

where H is a self-adjoint Hamiltonian and $E_1, E_2 \dots$ is the set of eigenvalues associat with a complete, discrete set $|1\rangle, |2\rangle, \dots$ of eigenvectors of H.

(a) denote the inner product of two states ψ, ϕ by $\langle\psi|\phi\rangle$. Prove that

$$\langle i|j\rangle = 0 \quad \text{if } E_i \neq E_j$$

let: $\langle i|H|j\rangle = E_i\langle i|j\rangle$ and $\langle i|H|j\rangle = E_j\langle i|j\rangle$
subtracting these two results yields

$$\langle i|H|j\rangle - \langle i|H|j\rangle = (E_i - E_j)\langle i|j\rangle$$

$$\Rightarrow \langle i|j\rangle(E_i - E_j) = 0$$

we immediately see that if $E_i \neq E_j$, then $\langle i|j\rangle = 0$ ✓

(b) Show that, if A is any well defined operator acting on the eigenstates, then the expectation value of $[A,H]$ on any eigenstate of H is zero.

$$\langle [A,H]\rangle = \langle i|[A,H]|i\rangle = \langle i|AH|i\rangle - \langle i|HA|i\rangle$$

$$= E_i\langle i|A|i\rangle - \langle i|H^{+}A|i\rangle \quad , \quad H = H^{+} \text{ since self-adjoint}$$

$$= E_i\langle i|A|i\rangle - E_i\langle i|A|i\rangle$$

$$\therefore \boxed{\langle [A,H]\rangle = 0}$$

(c) consider the case of a hydrogen atom. Use the statement in (b), with H the Schrödinger hydrogen atom Hamiltonian and A the dilation operator

$$A = \sum_{i=1}^{3} x_i \frac{d}{dx_i}$$

to prove that the expectation value of the kinetic energy in a bound state is equal to (the absolute zero of) the binding energy and the expectation value of the potential energy is -2 times as much.

From part (b), we know that $0 = \langle [A, H] \rangle$

$$\Rightarrow 0 = \langle i [A, T] | i \rangle + \langle i | [A, V] | i \rangle = 0 \qquad (1)$$

where $[A,T] = \left[\sum_i^3 x_i \frac{d}{dx_i}, \sum_j \frac{P_j^2}{2m} \right] = \frac{\hbar i}{2m}\left[\sum_i x_i P_i, \sum_j P_j^2 \right]$

$$\frac{d}{dx} = iP_x$$

this will vanish unless $i = j$. So, we have

$$[A,T] = \frac{+i}{2m} \sum_i [x_i P_i, P_i^2] = \frac{+i}{2m} \sum_i \left\{ P_i [x_i P_i, P_i] + [x_i P_i, P_i] P_i \right.$$

$$= \frac{+i}{2m} \sum_i \left\{ P_i x_i \cancelto{0}{[P_i, P_i]} + P_i \cancelto{i}{[x_i, P_i]} P_i + x_i \cancelto{0}{[P_i, P_i]} P_i + \right.$$

$$\left. + \cancelto{i}{[x_i, P_i]} P_i^2 \right\}$$

$$= \frac{+i}{2m} \sum_i \left\{ i P_i^2 + i P_i^2 \right\} = \frac{-2}{2m} \sum_i P_i^2 = -2T$$

Thus, $\boxed{[A,T] = -2T}$

and

$$[A, V] = \left[\sum_i x_i \frac{d}{dx_i}, V\right] = \sum_i \left\{ x_i \left[\frac{d}{dx_i}, V\right] + [x_i, V]\frac{d}{dx_i} \right\}$$

apply this to a state.

$$[A, V]\psi = \sum_i \left\{ x_i \frac{d}{dx_i} V\psi - x_i V \frac{d}{dx_i}\psi - x_i V \frac{d}{dx_i}\psi - V x_i \frac{d}{dx_i}\psi \right\}$$

$$= \sum_i \left\{ \psi x_i \frac{d}{dx_i} V + \underbrace{x_i V \frac{d}{dx_i}\psi - x_i V \frac{d}{dx_i}\psi}_{=0} + V x_i \frac{d}{dx_i}\psi \right\}$$

$$= \sum_i x_i \frac{d}{dx_i}(V\psi)$$

for hydrogen,

see other solution and Griffiths' 4.41 (Virial theorem)

$$[A, V] = r \cdot \nabla (V\psi) = -\langle V \rangle$$

Thus, going back to eq (1)

$$0 = -2\langle T \rangle - \langle V \rangle$$

$$\therefore \boxed{-2\langle T \rangle = \langle V \rangle}$$

Also,

$$\langle H \rangle = \langle T \rangle + \langle V \rangle = -\frac{1}{2}\langle V \rangle + \langle V \rangle = \frac{1}{2}\langle V \rangle$$

$$\therefore \boxed{E = 2\langle V \rangle}$$

or

$$\boxed{E = -\langle T \rangle}$$