

Spring 1997 #10 (p 1 of 3)

Consider a Schrödinger eigenvalue Problem of the form

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

where H is a self-adjoint Hamiltonian and E_1, E_2, \dots is the set of eigenvalues associated 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.

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

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

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

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

(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 $0 = \langle [A, H] \rangle$

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

where $[A, T] = \left[\sum_i x_i \frac{d}{dx_i}, \sum_j \frac{p_j^2}{2m} \right] = \frac{i}{2m} \left[\sum_i x_i p_i, \sum_j p_j^2 \right]$

$$\frac{d}{dx} = i p_x$$

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

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

$$= \frac{i}{2m} \sum_i \left\{ p_i x_i [p_i, p_i] + p_i [x_i, p_i] p_i + x_i [p_i, p_i] p_i + [x_i, p_i] p_i^2 \right\}$$

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

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

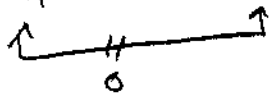
and

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

apply this to a state.

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

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



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

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

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