Spring 1997 #10

Consider a Schrödinger eigenvalue problem of the form

$$H|i\rangle = E_i|i\rangle \qquad i=1,2,\cdots$$

where H is a self-adjoint Hamiltonian and $E_1, E_2 \cdots$ is the set of eigenvalues associated with a complete, discrete set $|1\rangle, |2\rangle, \cdots$ 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 H act on $|i\rangle, |j\rangle$

$$H|i\rangle = E_i|i\rangle \qquad H|j\rangle = E_j|j\rangle$$

now calculate $\langle i|H|j\rangle$

if H acts on j : $\langle i|H|j\rangle = E_j\langle i|j\rangle$ (i)

if H acts on i : $\langle i|H|j\rangle = E_i\langle i|j\rangle$ (ii)

subtract (i) − (ii) to yield

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

thus

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

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

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

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

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

(c) Consider the case of the Hydrogen atom. Use the statement in (b), with H the Schrödinger hydrogen atom (i.e. Coulomb interaction) Hamiltonian and A the dilation (scaling) operator $A = \sum_{i=1}^{3} x_i \frac{d}{dx_i}$ to prove that the expectation value of T is equal to the absolute value of the expectation value of E ($\langle T\rangle = |\langle E\rangle|$) and also $\langle V\rangle = -2\langle E\rangle$

→ from (b) we know $\langle [A,H] \rangle = 0$

$$\langle i | [A, T+V] | i \rangle = \langle i | [A,T] | i \rangle + \langle i | [A,V] | i \rangle = 0$$

calculate $[A,T] = \left[\sum_i x_i \frac{d}{dx_i}, \sum_j p_j^2/2m \right]$ ← nonzero only for $i=j$

calculate $x_i = x$ using $\frac{d}{dx_i} = \frac{i}{\hbar} p_x$

$$\frac{i}{2\hbar m}[x p_x, p_x^2] = \frac{i}{2m\hbar}\left(x [p_x, p_x^2] + [x, p_x^2] p_x \right) \quad ([p_x, p_x^2] = 0)$$

$$= \frac{i}{2m\hbar}\left(p_x \underbrace{[x, p_x]}_{i\hbar} p_x + [x, p_x] p_x^2 \right)$$

$$= -\frac{2}{2m} p_x^2 \qquad \Rightarrow [A,T] = -2T$$

recognize $A = r \cdot \nabla$ and calculate $[A,V]\psi$

$$[A,V]\psi = (AV - VA)\psi = r \cdot \nabla (V\psi) - V r \cdot \nabla \psi$$

$$= \vec{r} \cdot [(V \nabla \psi) + \psi \nabla V] - V r \cdot \nabla \psi$$

$$= \psi \vec{r} \cdot \nabla V$$

$$\nabla V = \frac{d}{dr}\left(\frac{Ce^2}{r}\right) = \frac{Ce^2}{r^2} \hat{r}$$

$$[A,V]\psi = \frac{Ce^2}{r^2} \psi \quad \Rightarrow [A,V] = -V$$

Thus,

$$\langle i | [A,T] | i \rangle + \langle i | [A,V] | i \rangle = 0$$

$$-2\langle T \rangle - \langle V \rangle = 0 \qquad \Rightarrow \boxed{-2\langle T \rangle = \langle V \rangle}$$

Now $\langle H \rangle = \langle T \rangle + \langle V \rangle = \langle E \rangle$

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

$$\frac{1}{2}\langle V \rangle = \langle E \rangle$$

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