176(2): Application of the Quantum Hamilton Equations, Part 1

For any operator $\hat{A}$ and any wave function of quantum mechanics and relativistic quantum mechanics, and quantum optics and quantum field theory, the two quantum Hamilton equations are:

$$\frac{d\langle\hat{A}\rangle}{dx} = \frac{i}{\hbar}\langle[\hat{p}, \hat{A}]\rangle \quad -(1)$$

and

$$\frac{d\langle\hat{A}\rangle}{dp} = -\frac{i}{\hbar}\langle[\hat{x}, \hat{A}]\rangle. \quad -(2)$$

These are powerful new equations of quantum mechanics

when

$$\hat{A} = \hat{H} \quad -(3)$$

where $\hat{H}$ is the Hamiltonian operator, then:

$$\frac{d}{dx}\langle\hat{H}\rangle = \frac{i}{\hbar}\langle[\hat{p}, \hat{H}]\rangle \quad -(4)$$

$$\frac{d}{dp}\langle\hat{H}\rangle = -\frac{i}{\hbar}\langle[\hat{x}, \hat{H}]\rangle. \quad -(5)$$

The $\hat{H}$ operator is:

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x), \quad -(6)$$

so

$$[\hat{x}, \hat{H}]\psi = \hat{x}(\hat{H}\psi) - \hat{H}(\hat{x}\psi)$$

$$= x\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)\psi - \left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)\right)(x\psi)$$

2) $$= -x \frac{\hbar^2}{2m}\frac{\partial^2 \phi}{\partial x^2} + \frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}(x\phi). \quad -(7)$$

Here:

$$\frac{\partial^2}{\partial x^2}(x\phi) = \frac{\partial}{\partial x}\left(\frac{\partial(x\phi)}{\partial x}\right) = \frac{\partial}{\partial x}\left(\phi + x\frac{\partial \phi}{\partial x}\right) \quad -(8)$$

$$= 2\frac{\partial \phi}{\partial x} + x\frac{\partial^2 \phi}{\partial x^2}.$$

$$-(9)$$

So $$[\hat{x}, \hat{H}]\phi = \frac{\hbar^2}{m}\frac{\partial \phi}{\partial x}$$

i.e. $$\frac{d\langle \hat{H}\rangle}{dp} = -i\frac{\hbar}{m}\left\langle\frac{\partial \phi}{\partial x}\right\rangle = \frac{p}{m} \quad -(10)$$

By quantum classical equivalence:

$$\boxed{\frac{dH}{dp} = \frac{p}{m} = v} \quad -(11)$$

in non-relativistic classical dynamics. Note carefully that this result is true for all $V(x)$.

Similarly:

$$[\hat{p}, \hat{H}]\phi = -i\hbar\frac{\partial}{\partial x}(\hat{H}\phi) + i\hbar\hat{H}\frac{\partial \phi}{\partial x} \quad -(12)$$

$$= -i\hbar\frac{\partial}{\partial x}\left(\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\phi\right) + i\hbar\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V\right)\frac{\partial \phi}{\partial x}$$

$$= -i\hbar\frac{\partial}{\partial x}(V\phi) + i\hbar V\frac{\partial \phi}{\partial x} = -i\hbar\frac{\partial V}{\partial x}\phi$$

3)

$$[\hat{p}, \hat{H}]\phi = -i\hbar \frac{\partial V}{\partial x}\phi \quad -(13)$$

and

$$\boxed{\langle [\hat{p}, \hat{H}] \rangle = -i\hbar \frac{\partial V}{\partial x}} \quad -(14)$$

Therefore from eq. (14) & eq. (4):

$$\frac{d\langle \hat{H} \rangle}{dx} = \frac{\partial V}{\partial x}. \quad -(15)$$

From quantum classical equivalence:

$$\boxed{\frac{dH}{dx} = \frac{\partial V}{\partial x}} \quad -(16)$$

The two equations (4) and (5) are linked by the equation of motion:

$$\frac{d}{dt}\langle \hat{A} \rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{A}] \rangle, \quad -(17)$$

so when:

$$\hat{A} = \hat{H} \quad -(18)$$

$$\frac{d\langle \hat{H} \rangle}{dt} = 0. \quad -(19)$$

From eqs (1) and (2):

$$\boxed{\frac{d\langle \hat{p} \rangle}{dx} = \frac{d\langle \hat{x} \rangle}{dp} = 0} \quad -(20)$$

and x and p are <u>independent</u> variables.

4)

Any valid hamiltonian of quantum mechanics obeys eqs. (1), (2) and (17). From eq. (16), the force is:

$$F = -\frac{\partial V}{\partial x} = -\frac{dH}{dx} \quad - \left(\overset{21}{\cancel{17}}\right)$$

and if a system is being considered where there is no potential energy, for example free rotational and translational motion, then:

$$\frac{dH}{dx} = 0. \quad - \left(\overset{22}{\cancel{18}}\right)$$

The two classical Hamilton equations are:

$$\frac{dH}{dx} = -\frac{dp}{dt} \quad - \left(\overset{23}{\cancel{19}}\right)$$

and

$$\frac{dH}{dp} = \frac{dx}{dt}. \quad - \left(\overset{24}{\cancel{20}}\right)$$

Comparing eqs. (11) and (24):

$$v = \frac{dx}{dt} \quad - \left(\overset{25}{\cancel{21}}\right)$$

Q.E.D., and comparing eqs. $\left(\overset{21}{\cancel{17}}\right)$ and $\left(\overset{23}{\cancel{19}}\right)$:

$$F = m\frac{d^2v}{dt^2} \quad - \left(\overset{26}{\cancel{22}}\right)$$

which is Newton's law, Q.E.D.

Differentiating eq. (1) gives:

$$\frac{d^2}{dx^2}\langle x^2\rangle = 2 = \frac{i}{\hbar}\frac{\partial}{\partial x}\langle[\hat{p}, \hat{x}^2]\rangle \quad - \left(\overset{27}{\cancel{23}}\right)$$

So:

$$\frac{d^2}{dx^2}\langle \hat{A}^2 \rangle = \frac{i}{\hbar}\frac{\partial}{\partial x}\langle [\hat{p}, \hat{A}^2] \rangle \quad -\left(\overset{28}{\cancel{24}}\right)$$

here $\hat{A}^2$ is <u>any</u> <u>valid</u> <u>operator</u> <u>of quantum mechanics.</u>

Therefore:

$$\boxed{\frac{d^n}{dx^n}\langle \hat{A}^n \rangle = \frac{i}{\hbar}\frac{\partial}{\partial x^{n-1}}\langle [\hat{p}, \hat{A}^n] \rangle} \quad -\left(\overset{29}{\cancel{25}}\right)$$

and:

$$\boxed{\frac{d^n}{dp^n}\langle \hat{A}^n \rangle = -\frac{i}{\hbar}\frac{\partial}{\partial p^{n-1}}\langle [\hat{x}, \hat{A}^n] \rangle} \quad -\left(\overset{30}{\cancel{26}}\right)$$

For example, $\langle [\hat{p}, \hat{x}^2] \rangle = -2i\hbar x \quad -\left(\overset{31}{\cancel{27}}\right)$

and $$\frac{d^2}{dx^2}\langle x^2 \rangle = \frac{i}{\hbar}\left(-2i\hbar\frac{dx}{\partial x}\right) = 2 \quad -\left(\overset{32}{\cancel{28}}\right)$$

<u>Q.E.D.</u>