

177(1) : Derivation of Quantum Force Equation from Schrodinger Equation.

Consider the Schrodinger equation:

$$\hat{H}\psi = E\psi \quad - (1)$$

then

$$\frac{d}{dx}(\hat{H}\psi) = \frac{d}{dx}(E\psi) \quad - (2)$$

$$= E \frac{d\psi}{dx} \quad - (3)$$

because the energy levels  $E$  are independent of  $x$ .

Therefore:  $\left(\frac{d\hat{H}}{dx}\right)\psi + \hat{H}\frac{d\psi}{dx} = E\frac{d\psi}{dx} \quad - (4)$

The Hamiltonian is:

$$H = \frac{p^2}{2m} + V(x) \quad - (5)$$

so  $\frac{dH}{dx} = \frac{dV(x)}{dx} \quad - (6)$

because  $p$  and  $x$  are independent. Therefore:

$$\frac{dH}{dx} = \left\langle \frac{d\hat{H}}{dx} \right\rangle = \frac{dV(x)}{dx} \quad - (7)$$

$$= -F$$

from eqs. (4) and (7):

$$-F\psi + \hat{H}\frac{d\psi}{dx} = E\frac{d\psi}{dx} \quad - (8)$$

2) Therefore:

$$\hat{H} \frac{d\psi}{dx} = E \frac{d\psi}{dx} + F\psi \quad - (9)$$

where

$$\hat{H} = -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V(x) \quad - (10)$$

Eq. (9) is a very useful force equation because it uses the Schrodinger energy levels and wave functions.

Using computer algebra, the force energy levels can now be worked out for any problem in quantum mechanics.

The quantum hamilton equation is:

$$i\hbar \frac{d}{dx} \langle \hat{H} \rangle = \langle [\hat{H}, \hat{p}] \rangle \quad - (11)$$

where

$$\langle [\hat{H}, \hat{p}] \rangle = i\hbar \frac{dV}{dx} \quad - (12)$$

so

$$\frac{d\langle \hat{H} \rangle}{dx} = \frac{dH}{dx} = \frac{dV}{dx} = -F = -\frac{dp}{dt} \quad - (13)$$

This result checks eq. (6).

The fundamental rule energy that

$$\frac{d}{dx} \left( \frac{p^2}{2m} \right) = 0 \quad - (14)$$

3) because in Hamilton's dynamics,  $p$  and  $x$  are independent. So although:

$$\frac{\hat{p}^2}{2m} \psi = -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \quad - (15)$$

eq. (14) is still true, where:

$$\frac{p^2}{2m} = \left\langle \frac{\hat{p}^2}{2m} \right\rangle, \quad - (16)$$

so

$$\boxed{\frac{d}{dx} \left\langle \frac{\hat{p}^2}{2m} \right\rangle = 0} \quad - (17)$$

This means:

$$\boxed{-\frac{\hbar^2}{2m} \frac{d}{dx} \int \psi^* \frac{\partial^2 \psi}{\partial x^2} d\tau = 0} \quad - (18)$$

In eq. (11):

$$\begin{aligned} \frac{d}{dx} \langle \hat{H} \rangle &= -\frac{\hbar^2}{2m} \frac{d}{dx} \int \psi^* \frac{\partial^2 \psi}{\partial x^2} d\tau + \int \psi^* \frac{dV}{dx} \psi d\tau \\ &= \left\langle \frac{dV}{dx} \right\rangle \quad - (19) \\ &= \frac{dV}{dx} \end{aligned}$$

In general:

$$\left\langle \frac{d\hat{H}}{dx} \right\rangle = \int \psi^* \frac{d\hat{H}}{dx} \psi d\tau \quad - (20)$$

4) From eq. (17):

$$\left\langle \frac{d\hat{H}}{dx} \right\rangle = \frac{d\langle \hat{H} \rangle}{dx} \quad - (21)$$

as used in HFT 176. This is because:

$$\int \psi^* \frac{d\hat{H}}{dx} \psi d\tau = -\frac{\hbar^2}{2m} \int \psi^* \frac{\partial^2}{\partial x^2} \psi d\tau + \int \psi^* \frac{dV}{dx} \psi d\tau \quad - (22)$$

$$= \int \psi^* \frac{dV}{dx} \psi d\tau = \frac{dV}{dx} = \frac{d\langle \hat{H} \rangle}{dx}$$

A.E.D.

Because of the independence of  $x$  and  $p$  it follows that:

$$\left( \frac{d}{dx} \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \right) \right) \psi = 0 \quad - (23)$$

In general:

$$\left( \frac{d}{dq} \left( -\frac{\hbar^2}{2m} \frac{\partial^2}{\partial q^2} \right) \right) \psi = 0 \quad - (24)$$

because of the correspondence between Hamiltonian and momentum operators:

$$\boxed{\left( \frac{d}{dx} \left( -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} \right) \right) = \left( \frac{d}{dx} \left( \frac{p^2}{2m} \right) \right) \psi = 0} \quad - (25)$$

# 5) Summary Appendix

$$H = \frac{p^2}{2m} + V(q) \quad - (1)$$

$$\frac{dH}{dq} = \frac{dV}{dq} \quad - (2)$$

$$\text{So } \left( \frac{d\hat{H}}{dq} \right) \psi = \frac{dV}{dq} \psi \quad - (3)$$

The operator  $d\hat{H}/dq$  has no  $p$  dependence, so acts in a similar manner to:

$$\hat{x} \psi = x \psi \quad - (4)$$

From the Schrodinger equation it follows that:

$$\frac{d}{dx} (\hat{H} \psi) = \frac{d}{dx} (E \psi) = E \frac{d\psi}{dx} \quad - (5)$$

$$\text{So } \left( \frac{d\hat{H}}{dx} \right) \psi + \hat{H} \left( \frac{d\psi}{dx} \right) = E \frac{d\psi}{dx} \quad - (6)$$

$$\text{where } \left( \frac{d\hat{H}}{dx} \right) \psi = \left( \frac{dV}{dx} \right) \psi = -F \psi \quad - (7)$$

$$\text{So: } \boxed{\hat{H} \left( \frac{d\psi}{dx} \right) = F \psi + E \frac{d\psi}{dx}} \quad - (8)$$

And is eq (9) of the note, QED.