1) 175(15):

Proof of the Quantum Hamilton Equations

: The position representation gives the first Hamilton equation, and the momentum representation the second Hamilton equation.

Position Representation

$$\hat{p}_x \phi = -i\hbar \frac{\partial \phi}{\partial x}, \quad \hat{x}\phi = x\phi \qquad -(1)$$

$$\hat{p}_x^* \phi^* = i\hbar \frac{\partial \phi^*}{\partial x}, \quad \hat{x}\phi^* = x\phi^*$$

$$\frac{\partial \phi}{\partial x} = -\frac{\hat{p}}{i\hbar}\phi, \quad \frac{\partial \phi^*}{\partial x} = \frac{\hat{p}^*}{i\hbar}\phi^* \qquad -(2)$$

Momentum Representation

$$\hat{x}\phi = -\frac{\hbar}{i}\frac{\partial \phi}{\partial p_x}, \quad \hat{p}_x \phi = p_x \phi \qquad -(3).$$

$$\hat{x}^* \phi^* = \frac{\hbar}{i}\frac{\partial \phi^*}{\partial p_x}, \quad \hat{p}_x \phi^* = p_x \phi^*$$

$$\frac{\partial \phi}{\partial p_x} = \frac{\hat{x}}{i\hbar}\phi; \quad \frac{\partial \phi^*}{\partial p_x} = -\frac{\hat{x}^*}{i\hbar}\phi^* \qquad -(4)$$

First Quantum Hamilton Equation

First note that the definition of hermiticity is:

$$\int \phi_n^* \Omega \phi_n \, d\tau = \left(\int \phi_n^* \Omega \phi_n \, d\tau\right)^* = \int \phi_n \Omega^* \phi_n^* \, d\tau \qquad -(5)$$

Now use: $\int \phi_n \Omega^* \phi_n^* \, d\tau = \int \Omega^* \phi_n^* \phi_n \, d\tau \qquad -(6)$

This proves the Atkins result (5.2.2).

) Now consider:

$$\hat{p}\psi = -i\hbar \frac{\partial \psi}{\partial x} \quad , \quad (\hat{p}\psi)^* = i\hbar \frac{\partial \psi^*}{\partial x} \quad -(7)$$

Therefore:

$$\frac{d\langle \hat{x} \rangle}{dx} = 1 = -\frac{d}{dx}\int \psi^* \hat{x} \psi \, d\tau$$

$$= -\left(\int \frac{\partial \psi^*}{\partial x} \hat{x} \psi \, d\tau + \int \psi^* \hat{x} \frac{\partial \psi}{\partial x} \, d\tau \right)$$

$$= \frac{i}{\hbar} \int (\hat{p}\psi)^* \hat{x} \psi - \psi^* \hat{x}\hat{p} \psi \, d\tau \quad -(8)$$

From eq. (6):

$$\frac{d\langle \hat{x} \rangle}{dx} = 1 = \frac{i}{\hbar}\int \psi^* (\hat{p}\hat{x} - \hat{x}\hat{p}) \psi \, d\tau$$

$$= \frac{i}{\hbar}\int \psi^* [\hat{p}, \hat{x}] \psi \, d\tau$$

$$\frac{d\langle \hat{x} \rangle}{dx} = \frac{i}{\hbar} \langle [\hat{p}, \hat{x}] \rangle \quad -(9)$$

The first quantum Hamilton equation is obtained by generalizing:

$$\hat{x} \rightarrow \hat{A} \quad -(10)$$

and is:

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

where $\langle \hat{A} \rangle$ is <u>any</u> <u>operator</u>.

3) So if: $\hat{A} = \hat{H}$ $-(12)$

where $\hat{H}\phi = E\phi$ $-(13)$

then:

$$\frac{d}{dx}\langle \hat{H} \rangle = \frac{i}{\hbar}\langle [\hat{p}, \hat{H}] \rangle \quad -(14)$$

However, it is known that:

$$\frac{d}{dt}\langle \hat{p} \rangle = \frac{i}{\hbar}\langle [\hat{H}, \hat{p}] \rangle \quad -(15)$$

so the first quantum Hamilton equation is:

$$\boxed{\frac{d}{dx}\langle \hat{H} \rangle = -\frac{d}{dt}\langle \hat{p} \rangle} \quad -(16)$$

i.e.

$$\frac{dH}{dx} = -\frac{dp}{dt}, \quad -(17)$$

Q.E.D

Check

when $\hat{A} = \hat{x}^2$ $-(18)$

$$\langle [\hat{p}, \hat{x}^2] \rangle = -i\hbar \frac{dx^2}{dx} = -2i\hbar x. \quad -(19)$$

This is correct because:

$$[\hat{p}, \hat{x}^2]\phi = [\hat{p}, \hat{x}\hat{x}]\phi = -\left([\hat{x}, \hat{p}]\hat{x} + \hat{x}[\hat{x}, \hat{p}]\right)\phi = -2i\hbar x \quad -(20)$$

Q.E.D.

4)

: Note carefully that in order to obtain the correct result, then:

$$\langle x \rangle = x \quad -(21)$$

but a minus sign enters into the right hand side of eq. (8).

When:

$$\hat{A} = \hat{p} \quad -(22)$$

then:

$$\frac{d\langle \hat{p} \rangle}{dx} = 0 \quad -(23)$$

i.e. $\langle \hat{p} \rangle = p$ does not change with distance:

$$\boxed{\frac{dp}{dx} = 0} \quad -(24)$$

is a classical result. The minus sign in eq. (8) is a fundamental axiom of quantum mechanics:

$$\boxed{\frac{d\langle \hat{x} \rangle}{dx} = -\frac{d}{dx}\int \psi^* \hat{x} \psi \, d\tau = 1} \quad -(25)$$

Second Quantum Hamilton Equation.

By axiom:

$$\boxed{\frac{d\langle \hat{p} \rangle}{dp} = -\frac{d}{dp}\int \psi^* \hat{p} \psi \, d\tau = 1} \quad -(26)$$

$$= -\int \left(\frac{\partial \psi^*}{\partial p} \hat{p} \psi + \psi^* \hat{p} \frac{\partial \psi}{\partial p} \right) d\tau \quad -(27)$$

5) Using eq. (4):

$$\frac{d\langle\hat{p}\rangle}{dp} = 1 = \frac{1}{i\hbar}\int\left(\hat{x}^{*}\psi^{*}\hat{p}\psi - \psi^{*}\hat{p}\hat{x}\psi\right)d\tau \quad -(28)$$

Using eq. (5):

$$\frac{d\langle\hat{p}\rangle}{dp} = 1 = \frac{1}{i\hbar}\int\psi^{*}\left(\hat{x}\hat{p} - \hat{p}\hat{x}\right)\psi\, d\tau \quad -(29)$$

$$= -\frac{i}{\hbar}\langle[\hat{x},\hat{p}]\rangle \quad -(30)$$

Generalizing: $\hat{p} \rightarrow \hat{A}$. $-(31)$

So:

$$\boxed{\frac{d\langle\hat{A}\rangle}{dp} = -\frac{i}{\hbar}\langle[\hat{x},\hat{A}]\rangle} \quad -(32)$$

<u>for any $\hat{A}$.</u>

<u>Check</u>

If $\hat{A} = \hat{p}^2$ then:

$$\langle[\hat{x},\hat{p}^2]\rangle = 2ip\hbar. \quad -(33)$$

This is correct because:

$$[\hat{p}^2,\hat{x}]\psi = [\hat{p}\hat{p},\hat{x}]\psi$$
$$= -\left([\hat{x},\hat{p}]\hat{p} + \hat{p}[\hat{x},\hat{p}]\right)\psi \quad -(34)$$
$$= -2i\hbar p$$

Q.E.D

Now consider:

6)

$$\hat{A} = \hat{H} \quad -(35)$$

then:

$$\boxed{\frac{d}{dp}\langle \hat{H} \rangle = -\frac{i}{\hbar}\langle [\hat{x}, \hat{H}] \rangle} \quad -(36)$$

which is the second quantum Hamilton equation.

It is known that:

$$\langle [\hat{x}, \hat{H}] \rangle = -\frac{\hbar}{i}\frac{d}{dt}\langle \hat{x} \rangle \quad -(37)$$

so

$$\boxed{\frac{d}{dp}\langle \hat{H} \rangle = \frac{d}{dt}\langle \hat{x} \rangle} \quad -(38)$$

i.e

$$\frac{dH}{dp} = \frac{dx}{dt} \quad -(39)$$

which is Hamilton's second equation in classical dynamics, Q.E.D.