Motion of Q, i.e. $(d/dt)\langle Q\rangle$, as determined by $\mathcal{H}$.

The Quantum-Mechanical Equation-of-Motion.

In Schrödinger's Eqtn: $i\hbar\,\partial\psi/\partial t = \mathcal{H}\psi$, the Hamiltonian operator $\mathcal{H}$ specifies how the wavefcn ψ evolves in time. In turn, ψ specifies the time-dependence of a ; quantity Q via the expectation value $\langle Q\rangle = \langle\psi|Q\psi\rangle$. Thus, we anticipate that there is a relationship between $\mathcal{H}$ and Q's dependence on time -- in particular, $\mathcal{H}$ should determine the time dependence of Q. We now show this is the case by analysing how a general operator $Q = Q(\mathbf{r}, \mathbf{p}, t)$ evolves in time, in an expectation value sense (of course).

1) For $Q = Q(\mathbf{r}, \mathbf{p}, t)$, the expectation value is $\langle Q\rangle = \langle\psi|Q\psi\rangle$, and so...

$$\rightarrow \frac{d}{dt}\langle Q\rangle = \langle(\tfrac{\partial\psi}{\partial t})|Q\psi\rangle + \underbrace{\langle\psi|(\tfrac{\partial Q}{\partial t})\psi\rangle}_{=\langle\partial Q/\partial t\rangle} + \langle\psi|Q(\tfrac{\partial\psi}{\partial t})\rangle \tag{1}$$

$\partial\psi/\partial t = -\frac{i}{\hbar}\mathcal{H}\psi$ $\qquad$ $\partial\psi/\partial t = -\frac{i}{\hbar}\mathcal{H}\psi$

$$= \langle\partial Q/\partial t\rangle + \frac{i}{\hbar}\underbrace{\langle\mathcal{H}\psi|Q\psi\rangle}_{=\langle\psi|\mathcal{H}(Q\psi)\rangle,\ \text{since } \mathcal{H} \text{ is Hermitian;}} - \frac{i}{\hbar}\langle\psi|Q(\mathcal{H}\psi)\rangle$$

So//

$$\rightarrow \frac{d}{dt}\langle Q\rangle = \left\langle\frac{\partial Q}{\partial t}\right\rangle + \frac{i}{\hbar}\langle\psi|\mathcal{H}(Q\psi) - Q(\mathcal{H}\psi)\rangle. \tag{2}$$

For a general product operator $C = AB$, let $B\psi = \phi$. So $C\psi = A\phi$, that is: $(AB)\psi = A(B\psi)$. Use this fact in (2) to write...

$$\frac{d}{dt}\langle Q\rangle = \left\langle\frac{\partial Q}{\partial t}\right\rangle + \frac{i}{\hbar}\langle\psi|(\mathcal{H}Q - Q\mathcal{H})\psi\rangle. \tag{3}$$

The combination in ( ) in Eq. (3) occurs often in QM. It is called...

$$\left[\!\!\left[\begin{matrix}\text{COMMUTATOR of}\\ \text{operators } A \,\&\, B\end{matrix}\right\}(AB - BA) \equiv [A,B] \leftarrow \boxed{\text{notation}}. \tag{4}$$

So// $\frac{d}{dt}\langle Q\rangle = \langle\partial Q/\partial t\rangle + (i/\hbar)\langle[\mathcal{H}, Q]\rangle$,

or// $\frac{d}{dt}Q = \frac{\partial Q}{\partial t} + (i/\hbar)[\mathcal{H}, Q]$, in an expectation value sense. $\qquad$ (5)

Q as a "constant-of-the-motion". Notes on commutators.

From Eq. (5), we see that apart from an explicit (built-in) dependence on time (i.e. $\partial Q/\partial t \neq 0$), the evolution of Q is in fact determined by $\mathcal{H}$, via the commutator $[\mathcal{H}, Q]$. The necessary and sufficient condition that $\langle Q\rangle$ is conserved -- i.e. is a "constant-of-the-motion", w/ $\frac{d}{dt}\langle Q\rangle = 0$ -- is...

$$\boxed{\text{For time-independent operators } Q \text{ (w/ } \partial Q/\partial t = 0\text{), } Q \text{ is a "constant-of-the-motion", i.e. } \frac{d}{dt}\langle Q\rangle = 0, \text{ if and only if } [\mathcal{H}, Q] = 0.} \tag{6}$$

Eq. (6) $\Rightarrow$ an easy way to find "constants-of-the-motion": calculate $[\mathcal{H}, Q]$.

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2) A note on commutators is in order. They are meant to be evaluated w.r.t. a wavefcn ψ, i.e. they should operate on some ψ. Thus $[A,B]$ by itself may have no meaning, but $[A,B]\psi$ does have the operational def$^{\underline{n}}$:

$$\rightarrow [A,B]\psi = A(B\psi) - B(A\psi). \tag{7}$$

A simple example is the commutator for position & momentum...

$$\rightarrow [x, p_x]\psi = x\left(-i\hbar\frac{\partial}{\partial x}\right)\psi - \left(-i\hbar\frac{\partial}{\partial x}\right)(x\psi)$$

$$= i\hbar\left[\frac{\partial}{\partial x}(x\psi) - x\frac{\partial\psi}{\partial x}\right] = i\hbar(\psi),$$

So// $\underline{\underline{[x, p_x] = i\hbar}}$, in an expectation value sense. (8)

By itself: $[x, p_x] = -i\hbar x\frac{\partial}{\partial x} + i\hbar\frac{\partial}{\partial x}x$, is not transparent... however, $[x, p_x]\psi$ is clear. More generally than (8), for position & momentum components x_k & p_l (k & $l = 1, 2, 3$), we can show...

$$\boxed{[x_k, p_l] = i\hbar\,\delta_{kl}}, \text{ w/ } \delta_{kl} = \begin{cases} 1, & \text{when } k = l; \\ 0, & \text{otherwise.} \end{cases} \text{ (Kronecker delta).} \tag{9}$$

The commutator $[x, p_x] = i\hbar$ is easily generalized to $x \to f(x)$, an arbitrary fcn of x...

Generalized Commutators w.r.t. x & p_x.

$\rightarrow [f(x), p_x]\psi = i\hbar\left[\frac{\partial}{\partial x}(f\psi) - f\frac{\partial\psi}{\partial x}\right] = \left(i\hbar\frac{\partial f}{\partial x}\right)\psi,$

i.e.// $\underline{\underline{[f(x), p_x] = i\hbar(\partial f/\partial x)}}$, in an expectation value sense. (10)

Also, since p_x commutes with itself (i.e. $[p_x, p_x] \equiv 0$) and all powers of itself:

$\boxed{[f(x, p_x), p_x] = i\hbar\frac{\partial}{\partial x}f(x, p_x)}$, in exp$^{\underline{n}}$ value sense. (11A)

The companion relation is ...

$\boxed{[x, F(x, p_x)] = i\hbar\frac{\partial}{\partial p_x}F(x, p_x)}$, in exp$^{\underline{n}}$ value sense. (11B)

We now prove (11B). Since x commutes with itself and all powers of itself, (11B) will be true for all F's that can be expanded in power series in p_x if we can show: $\underline{[x, p_x^n]} = i\hbar\frac{\partial}{\partial p_x}\underline{p_x^n}$, for all $n = 1, 2, 3, \ldots$ We can establish this proposition by mathematical induction...

Let $p_x = p$, as a shorthand.

$\underline{\underline{1.}}$ $[x, p^n] = i\hbar\frac{\partial}{\partial p}p^n$, is evidently true for $n=1$ (i.e. $[x,p] = i\hbar$). (12A)

$\underline{\underline{2.}}$ Assume true for n, i.e. $\underline{\underline{[x, p^n] = i\hbar\frac{\partial}{\partial p}p^n = i\hbar n p^{n-1}}}$.

Now -- from this assumption -- show proposition is true for $(n+1)$, i.e. show that: $[x, p^{n+1}] = i\hbar\frac{\partial}{\partial p}p^{n+1} = i\hbar(n+1)p^n$. (12B)

$\underline{\underline{3.}}$ Use a general commutator identity for a product operator (see problems):

$\rightarrow [A, BC] = B[A, C] + [A, B]C$;

so// $[x, p^{n+1}] = [x, p^n p] = p^n\underbrace{[x, p]}_{= i\hbar,\text{ by Eq. (8)}} + \underbrace{[x, p^n]}_{= i\hbar n p^{n-1},\text{ by assumption in } \underline{\underline{2}}}p$

$= i\hbar(p^n + np^{n-1}p) = i\hbar(n+1)p^n = i\hbar\frac{\partial}{\partial p}p^{n+1}$. QED (12C)

$\underline{\underline{4.}}$ $[x, p^n] = i\hbar(\partial/\partial p)p^n$, is true for $n=1$, and the assumption it is true for $n \Rightarrow$ it is true for $(n+1)$. By induction, it is true for $\underline{\text{all}}$ n.

This result, used judiciously in (11B), verifies that $[x, F(x,p)] = i\hbar \frac{\partial F}{\partial p}$.
Then for any operator $Q = Q(x,p,t)$, Eqs. (11A) & (11B) prescribe...

$$\boxed{[Q,p] = i\hbar(\partial Q/\partial x)\ ,\quad [x,Q] = i\hbar(\partial Q/\partial p)}\ . \quad \text{in an exp}^{\text{n}}\ \text{value sense.} \tag{13}$$

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3) Our QM Equation-of-Motion, i.e. Eq. (5) above (with $\exp^{\text{n}}$ values restored):

$$\boxed{\frac{d}{dt}\langle Q\rangle = \frac{i}{\hbar}\langle[\mathcal{H},Q]\rangle + \langle\partial Q/\partial t\rangle} \quad \mathcal{H} = \text{Hamiltonian operator, that generates wfcn } \Psi \text{ via: } \mathcal{H}\Psi = i\hbar\frac{\partial\Psi}{\partial t}. \tag{14}$$

Can be put to immediate good use. Namely, we can show that the eqtns-of-motion for position $\langle x\rangle$ and momentum $\langle p\rangle$ of a QM system (e.g. a particle of mass m) are just Hamilton's equations of classical mechanics...

$$\rightarrow \frac{d}{dt}\langle x\rangle = \frac{i}{\hbar}\langle\underbrace{[\mathcal{H},x]}_{\substack{= -i\hbar\,\partial\mathcal{H}/\partial p \\ \text{[2nd of Eqs. (13)]}}}\rangle + \underbrace{\cancelto{0}{\langle\partial x/\partial t\rangle}}_{\substack{x\,\&\,t \\ \text{are indept} \\ \text{variables}}} = +\langle\partial\mathcal{H}/\partial p\rangle; \tag{15A}$$

$$\rightarrow \frac{d}{dt}\langle p\rangle = \frac{i}{\hbar}\langle\underbrace{[\mathcal{H},p]}_{\substack{= +i\hbar\,\partial\mathcal{H}/\partial x \\ \text{[1st of Eqs. (13)].}}}\rangle + \underbrace{\cancelto{0}{\langle\partial p/\partial t\rangle}}_{\substack{p\,\&\,t \\ \text{are indept} \\ \text{variables}}} = -\langle\partial\mathcal{H}/\partial x\rangle; \tag{15B}$$

i.e.// in an expectation value sense: $\underline{\underline{\frac{d}{dt}x = \frac{\partial\mathcal{H}}{\partial p}\ ,\ \frac{d}{dt}p = -\frac{\partial\mathcal{H}}{\partial x}}}$. (15C)

Eqs. (15C) are just Hamilton's equations [ref. Ch. 6 of A. Fetter & J. Walecka, "Theoretical Mechanics of Particles & Continua" (McGraw-Hill, 1980)], and the QM expectation-value version is known as Ehrenfest's Theorem (1927). For a conservative system (no dissipation), $\mathcal{H}$ is a constant of the motion, and it may be identified with the system's total energy (K.E. + P.E.). If we write: $\mathcal{H} = p^2/2m + V(x)$, then Eqs. (15C) prescribe that: $\underline{\frac{d}{dt}x = p/m = v}$, $\underline{\frac{d}{dt}p = -\partial V/\partial x = F}$. In fact, we used these eqtns as input for our derivation of Schrödinger's Eqtn [ref p. Sch. 18 & 19, Eqs. (44) & (47)].