CEM 991 **Fall 2021**

Assignment No. 3 (25 pts.) **Due Date: October 15, 2021 (Friday)**

1. (6 pts.) The $1s$ and $2s$ states of the hydrogen atom are described by the wave functions

$$u_{1s}(r) = \frac{1}{\sqrt{\pi}} a_0^{-\frac{3}{2}} e^{-\frac{r}{a_0}}, \tag{1}$$

$$u_{2s}(r) = \frac{1}{\sqrt{32\pi}} a_0^{-\frac{3}{2}} (2 - \frac{r}{a_0}) e^{-\frac{r}{2a_0}}, \tag{2}$$

where r is the distance from the origin and a_0 is the radius of the first circular Bohr orbit.

   (a) Show that u_{1s} and u_{2s} are normalized to unity.

   (b) Compute the expectation value of r in the state described by u_{1s}.

   Auxiliary formula: $\int_0^\infty x^n e^{-\alpha x} dx = \frac{n!}{\alpha^{n+1}}$, $\alpha > 0$, $n = 0, 1, 2, \ldots$.

2. (4 pts.) The wave function of a freely moving particle in one dimension has the form,

$$\psi(x) = A e^{ikx}, \tag{3}$$

where A is a constant and $p = k\hbar$ is the momentum of a particle. Calculate the probability current density for this particle and compare the result with the equation from hydrodynamics,

$$\mathbf{j} = \rho \mathbf{v}, \tag{4}$$

where $\mathbf{j}$ and ρ are current density and density of the fluid, respectively, and $\mathbf{v}$ is the fluid velocity.$^{\#)}$

3. (7 pts.) Consider a three-dimensional wave packet $\psi = \psi(x, y, z, t)$ under the influence of a force derived from the real potential $V = V(x, y, z, t)$. The mass of the corresponding classical particle is designated by m. Show that

$$\frac{d}{dt}\langle \hat{L}_z \rangle = \langle \hat{D}_z \rangle, \tag{5}$$

where, in general,

$$\langle \hat{F} \rangle = \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} \psi^* \hat{F} \psi \, dx dy dz \tag{6}$$

represents the expectation value of the operator $\hat{F}$, $\hat{L}_z$ is the z component of the angular momentum operator, and

$$\hat{D}_z = \left(-\hat{x}\frac{\partial \hat{V}}{\partial y}\right) - \left(-\hat{y}\frac{\partial \hat{V}}{\partial x}\right). \tag{7}$$

Please comment on the result.
Hint: Use the fact that ψ represents a solution of the Schrödinger equation,

$$\imath\hbar\frac{\partial\psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\psi + V\psi, \tag{8}$$

and the property of the Laplacian,

$$\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\psi^*(\nabla^2\phi)dxdydz = \int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}\int_{-\infty}^{+\infty}(\nabla^2\psi)^*\phi dxdydz, \tag{9}$$

or the fact that the kinetic energy operator is Hermitian.

4. (8 pts.) Calculate the following commutators:

   (a) $[\hat{x}, \hat{p}_x^2]$,

   (b) $[\hat{x}^2, \hat{p}_x]$,

   (c) $[\hat{x}^2, \hat{p}_x^2]$

   ($\hat{p}_x$ is the x-component of the momentum operator $\hat{\mathbf{p}}$). Use (a)–(c) to evaluate the commutator $[\hat{x}, \hat{H}]$, where $H = \frac{p_x^2}{2m} + V(x)$ is the Hamiltonian.
   Hint: In evaluating the commutators (a)–(c), use the formula $[\hat{x}, \hat{p}_x] = \imath\hbar\mathbf{1}$, where $\mathbf{1}$ is the unit operator, and exploit properties of a commutator, such as $[\hat{F}_1\hat{F}_2, \hat{G}] = \hat{F}_1[\hat{F}_2, \hat{G}] + [\hat{F}_1, \hat{G}]\hat{F}_2$ (cf. Problem 5 of Assignment No. 2). In other words, use an algebraic approach.

#) Bold symbols designate vector quantities.

SOLUTIONS

1. (a) Normalization:

$$\int_{\mathbb{R}^3} u_{1s}^*(r)\, u_{1s}(r)\, \overset{dx\,dy\,dz}{d\tau} =$$

three-dimensional space (x, y, z)

depends on r only

Jacobian

$$= \int_0^\infty dr \int_0^\pi d\Theta \int_0^{2\pi} d\varphi \; u_{1s}(r)^2 \, \overbrace{r^2 \sin\Theta}^{\text{Jacobian}}$$

$$= \int_0^\infty u_{1s}(r)^2 r^2 dr \underbrace{\int_0^\pi \sin\Theta \, d\Theta \int_0^{2\pi} d\varphi}_{2 \times 2\pi = 4\pi} =$$

$$= 4\pi \int_0^\infty u_{1s}(r)^2 r^2 \, dr$$

$$= \cancel{4\pi} \frac{1}{\cancel{\pi}} a_0^{-3} \int_0^\infty e^{-\frac{2r}{a_0}} r^2 \, dr .$$

The last integral equals (cf. the auxiliary formula with $x = r$, $\alpha = \frac{2}{a_0}$, $n = 2$),

$$\int_0^\infty e^{-\frac{2r}{a_0}} r^2 \, dr = \frac{2!}{\left(\frac{2}{a_0}\right)^3} = \frac{2}{8} a_0^3$$

$$= \frac{1}{4} a_0^3 .$$

Thus

$$\int_{\mathbb{R}^3} u_{1s}^*(r) \, u_{1s}(r) \, d\tau =$$

$$= 4 \, a_0^{-3} \, \frac{1}{4} \, a_0^3 = 1 .$$

A very similar calculation for u_{2s} gives

$$\int_{\mathbb{R}^3} u_{2s}(r)^* u_{2s}(r)\, d\tau =$$

$$= \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\varphi \; u_{2s}(r)^2 r^2 \sin\theta$$

$$= 4\pi \int_0^\infty u_{2s}(r)^2 r^2\, dr$$

$$= 4\pi \frac{1}{32\pi} a_0^{-3} \int_0^\infty \left(2 - \frac{r}{a_0}\right)^2 e^{-\frac{r}{a_0}} r^2\, dr$$

$$= \frac{1}{8} a_0^{-3} \int_0^\infty \left(4 - \frac{4r}{a_0} + \frac{r^2}{a_0^2}\right) r^2 e^{-\frac{r}{a_0}} dr$$

$$= \frac{1}{8} a_0^{-3} \left\{ 4\int_0^\infty r^2 e^{-\frac{r}{a_0}} dr - \frac{4}{a_0}\int_0^\infty r^3 e^{-\frac{r}{a_0}} dr \right.$$

$$\left. + \frac{1}{a_0^2} \int_0^\infty r^4 e^{-\frac{r}{a_0}} dr \right\}$$

Now (cf. the auxiliary formula),

$$\int_0^\infty r^2 e^{-\frac{r}{a_0}} dr = \frac{2!}{\left(\frac{1}{a_0}\right)^3} = 2a_0^3 ,$$

$$\int_0^\infty r^3 e^{-\frac{r}{a_0}} dr = \frac{3!}{\left(\frac{1}{a_0}\right)^4} = 6a_0^4 ,$$

$$\int_0^\infty r^4 e^{-\frac{r}{a_0}} dr = \frac{4!}{\left(\frac{1}{a_0}\right)^5} = 24 a_0^5 .$$

Thus, $\displaystyle\int_{\mathbb{R}^3} u_{2s}(r)^* u_{2s}(r)\, d\tau =$

$$= \frac{1}{8} a_0^{-3} \left\{ 8a_0^3 - \cancel{24 a_0^3} + \cancel{24 a_0^3} \right\}$$

$$= \frac{1}{\cancel{8}} a_0^{-3} \cancel{8} a_0^3 = 1 .$$

$\therefore$

(b) The expectation value

$$\langle r \rangle_{1s} = \int_{\mathbb{R}^3} u_{1s}(r)^* \, r \, u_{1s}(r) \, d\tau$$

is

$$\langle r \rangle_{1s} = \int_0^\infty dr \int_0^\pi d\theta \int_0^{2\pi} d\varphi \; u_{1s}(r)^2 \, r^3 \sin\theta$$

$$= 4\pi \int_0^\infty u_{1s}(r)^2 \, r^3 \, dr$$

$$= 4\cancel{\pi} \frac{1}{\cancel{\pi}} a_0^{-3} \int_0^\infty e^{-\frac{2r}{a_0}} r^3 \, dr$$

$$= \frac{4}{a_0^3} \frac{3!}{\left(\frac{2}{a_0}\right)^4} = \frac{24}{a_0^{-1} \, 16} =$$

$$= \frac{3}{2} a_0 .$$

$$\langle r \rangle_{1s} = \frac{3}{2} a_0 .$$

2. $$S(x,t) = \frac{\hbar}{2im}\left(\psi^* \frac{\partial \psi}{\partial x} - \left(\frac{\partial \psi}{\partial x}\right)^* \psi\right)$$

defines the probability current density for all wave functions depending on x and t.

In our case,

$$\psi(x) = A e^{ikx}, \quad \psi^*(x) = A^* e^{-ikx}.$$

We obtain,

$$S(x,t) = \frac{\hbar}{2im}\Big(|A|^2 e^{-ikx}(ik)e^{ikx}$$

$$- |A|^2 (-ik)\, e^{-ikx} e^{ikx}\Big) = \frac{\hbar k}{m}|A|^2.$$

Note that $\frac{\hbar k}{m} = \frac{p}{m} = v$, where v is the velocity. Moreover, the probability density

$$\rho(x) = \psi^*(x)\psi(x) = A^* e^{-ikx} A e^{ikx}$$
$$= |A|^2 .$$

Thus, we have

$$S = \rho v .$$

In three dimensions, we would obtain,

$\vec{S} = \rho \vec{v}$, in complete analogy with the formula $\vec{j} = \rho \vec{v}$ known in hydrodynamics

3. $$\langle \hat{L}_z \rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi^* \hat{L}_z \psi \, dx\,dy\,dz$$

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

$$\langle \hat{L}_z \rangle = \frac{\hbar}{i}\iiint_{-\infty}^{\infty} \psi^* x \frac{\partial \psi}{\partial y} \, dx\,dy\,dz - \frac{\hbar}{i}\iiint_{-\infty} \psi^* y \frac{\partial \psi}{\partial x} dx\,dy\,dz$$

$$\frac{d}{dt}\langle \hat{L}_z \rangle = \frac{\hbar}{i}\iiint_{-\infty}^{\infty} \frac{\partial}{\partial t}\left(\psi^* x \frac{\partial \psi}{\partial y}\right) dx\,dy\,dz$$

$$- \frac{\hbar}{i}\iiint_{-\infty}^{\infty} \frac{\partial}{\partial t}\left(\psi^* y \frac{\partial \psi}{\partial x}\right) dx\,dy\,dz$$

$$= \frac{\hbar}{i}\iiint_{-\infty}^{\infty}\left[\frac{\partial \psi^*}{\partial t} x \frac{\partial \psi}{\partial y} + \psi^* x \frac{\partial}{\partial y}\frac{\partial \psi}{\partial t}\right] dx\,dy\,dz$$

$$- \frac{\hbar}{i}\iiint_{-\infty}^{\infty}\left[\frac{\partial \psi^*}{\partial t} y \frac{\partial \psi}{\partial x} + \psi^* y \frac{\partial}{\partial x}\frac{\partial \psi}{\partial t}\right] dx\,dy\,dz$$

From the Schrödinger equation,

$$\frac{\partial \psi}{\partial t} = -\frac{\hbar}{2mi}\nabla^2\psi + \frac{V}{i\hbar}\psi$$

$$\frac{\partial \psi^*}{\partial t} = \frac{\hbar}{2mi}\nabla^2\psi^* - \frac{V}{i\hbar}\psi^* \quad (V = V^*).$$

Thus,

$$\frac{d\langle \hat{L}_z\rangle}{dt} = \iiint_{-\infty}^{\infty}\left[\left(-\frac{\hbar^2}{2m}\left(\nabla^2\psi^*\right) + V\psi^*\right)x\frac{\partial\psi}{\partial y}\right.$$

$$\left. + \psi^* x \frac{\partial}{\partial y}\left(\frac{\hbar^2}{2m}\nabla^2\psi - V\psi\right)\right] dx\,dy\,dz$$

$$+ \iiint_{-\infty}^{\infty}\left[\left(\frac{\hbar^2}{2m}\nabla^2\psi^* - V\psi^*\right) y \frac{\partial\psi}{\partial x}\right.$$

$$\left. + \psi^* y \frac{\partial}{\partial x}\left(-\frac{\hbar^2}{2m}\nabla^2\psi + V\psi\right)\right] dx\,dy\,dz$$

$$= -\frac{\hbar^2}{2m}\left\{\iiint_{-\infty}^{\infty}\left(\nabla^2\psi^*\right)\left(x\frac{\partial\psi}{\partial y} - y\frac{\partial\psi}{\partial x}\right)dx\,dy\,dz\right.$$

$$\left. - \iiint_{-\infty}^{\infty}\psi^*\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\nabla^2\psi\, dx\,dy\,dz\right\}$$

$$+ \iiint_{-\infty}^{\infty} \Big[\cancel{(V\psi^*)\, x \frac{\partial \psi}{\partial y}} - \psi^* x \frac{\partial V}{\partial y} \psi$$

$$- \cancel{\psi^* x V \frac{\partial \psi}{\partial y}} \Big] \, dx\,dy\,dz$$

$$- \iiint_{-\infty}^{\infty} \Big[\cancel{(V\psi^*)\, y \frac{\partial \psi}{\partial x}} - \psi^* y \frac{\partial V}{\partial x} \psi$$

$$- \cancel{\psi^* y V \frac{\partial \psi}{\partial x}} \Big] \, dx\,dy\,dz \qquad (A)$$

Let us evaluate

$$\iiint_{-\infty}^{\infty} (\nabla^2 \psi^*) \left(x \frac{\partial \psi}{\partial y} - y \frac{\partial \psi}{\partial x} \right) dx\,dy\,dz .$$

From Eq. (9), we obtain

$$\iiint_{-\infty}^{\infty} (\nabla^2\psi^*)\left(x\frac{\partial\psi}{\partial y} - y\frac{\partial\psi}{\partial x}\right) dx\,dy\,dz$$

$$= \iiint_{-\infty}^{\infty} \psi^*\left(\nabla^2\left(x\frac{\partial\psi}{\partial y}\right) - \nabla^2\left(y\frac{\partial\psi}{\partial x}\right)\right) dx\,dy\,dz$$

Now,

$$\nabla^2\left(x\frac{\partial\psi}{\partial y}\right) - \nabla^2\left(y\frac{\partial\psi}{\partial x}\right) =$$

$$= \cancel{2\frac{\partial^2\psi}{\partial x\partial y}} + x\frac{\partial}{\partial y}(\nabla^2\psi)$$

$$- \cancel{2\frac{\partial^2\psi}{\partial y\partial x}} - y\frac{\partial}{\partial x}(\nabla^2\psi)$$

$$= \left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\nabla^2\psi.$$

Thus,

$$\iiint_{-\infty}^{\infty} (\nabla\psi^*)\left(x\frac{\partial\psi}{\partial y} - y\frac{\partial\psi}{\partial x}\right) dx\,dy\,dz$$

$$= \iiint_{-\infty}^{\infty} \psi^*\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)\nabla^2\psi \, dx\,dy\,dz.$$

The expression between { } in Eq. (A) above becomes zero and Eq. (A) reduces to

$$\frac{d\langle\hat{L}_z\rangle}{dt} = -\iiint_{-\infty}^{\infty}\left[\psi^* x\frac{\partial V}{\partial y}\psi - \right.$$

$$\left. - \psi^* y\frac{\partial V}{\partial x}\psi\right] dx\,dy\,dz$$

$$= -\iiint_{-\infty}^{\infty} \psi^*\left(x\frac{\partial V}{\partial y} - y\frac{\partial V}{\partial x}\right)\psi \, dx\,dy\,dz$$

$$= \iiint_{-\infty}^{\infty} \psi^* \hat{D}_z \psi \, dx\,dy\,dz = \langle \hat{D}_z \rangle,$$

which completes the calculation.

We could have performed an alternative calculation to obtain the same result, namely,

$$\frac{d\langle \hat{L}_z \rangle}{dt} = \iiint_{-\infty}^{\infty} \frac{\partial}{\partial t}\left(\psi^* \hat{L}_z \psi\right) dx\,dy\,dz$$

$$= \iiint_{-\infty}^{\infty} \left[\left(\frac{\partial \psi^*}{\partial t}\right) \hat{L}_z \psi - \cancelto{0}{\psi^* \frac{\partial \hat{L}_z}{\partial t} \psi} \right.$$

$$\left. + \psi^* \hat{L}_z \frac{\partial \psi}{\partial t} \right] dx\,dy\,dz \,.$$ From

the Schrödinger equation,

$$i\hbar \frac{\partial \psi}{\partial t} = \hat{H}\psi \,,$$ where

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V \,,$$ we obtain

$$\frac{\partial\psi}{\partial t} = \frac{1}{i\hbar}\hat{H}\psi, \quad \frac{\partial\psi^*}{\partial t} = -\frac{1}{i\hbar}\hat{H}\psi^*,$$

so that

$$\frac{d\langle\hat{L}_z\rangle}{dt} = \frac{1}{i\hbar}\iiint_{-\infty}^{\infty} \psi^*\left(\hat{L}_z\hat{H} - \hat{H}\hat{L}_z\right)\psi \, dx\,dy\,dz \qquad (B)$$

where we used that fact that

$$\iiint_{-\infty}^{\infty} \left(\frac{\partial\psi^*}{\partial t}\right)\hat{L}_z\psi \, dx\,dy\,dz =$$

$$= -\frac{1}{i\hbar}\iiint_{-\infty}^{\infty} \left(\hat{H}\psi^*\right)\hat{L}_z\psi \, dx\,dy\,dz$$

$$\underset{\text{hermitian}}{\overset{\hat{H}\text{ is}}{=}} -\frac{1}{i\hbar}\iiint_{-\infty}^{\infty} \psi^*\hat{H}\hat{L}_z\psi \, dx\,dy\,dz.$$

Eq. (7) plus the fact $\hat{V} = \hat{V}^*$

Thus, we must know (see Eq. (B))

$$\hat{L}_z \hat{H} - \hat{H}\hat{L}_z = [\hat{L}_z, \hat{H}].$$

It is easy to see that

$$[\hat{L}_z, \nabla^2] = 0$$ (please try yourself).

Thus,

$$[\hat{L}_z, \hat{H}] = [\hat{L}_z, \hat{V}] . \quad (C)$$

Let us calculate the latter expression,

$$[\hat{L}_z, \hat{V}]\psi = \frac{\hbar}{i}\left[\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)V\psi - V\left(x\frac{\partial\psi}{\partial y} - y\frac{\partial\psi}{\partial x}\right)\right]$$

$$= \frac{\hbar}{i}\left[x\frac{\partial V}{\partial y}\psi + \cancel{xV\frac{\partial\psi}{\partial y}} - y\frac{\partial V}{\partial x}\psi\right.$$

$$- y \cancel{V \frac{\partial \psi}{\partial x}} - \cancel{x V \frac{\partial \psi}{\partial y} + y V \frac{\partial \psi}{\partial x}} \Big]$$

$$= \frac{\hbar}{i}\left(x \frac{\partial V}{\partial y} - y \frac{\partial V}{\partial x}\right)\psi \quad \text{or}$$

unit operator

$$[\hat{L}_z, \hat{V}] = \frac{\hbar}{i}\left(x \frac{\partial V}{\partial y} - y \frac{\partial V}{\partial x}\right) 1 \qquad (D)$$

Returning to (B),

$$\frac{d\langle L_z\rangle}{dt} = \frac{1}{i\hbar}\iiint_{-\infty}^{\infty} \psi^* [\hat{L}_z, H]\psi \, dx\,dy\,dz$$

$$\overset{\text{Eq.(C)}}{=} \frac{1}{i\hbar}\iiint_{-\infty}^{\infty} \psi^* [\hat{L}_z, \hat{V}]\psi \, dx\,dy\,dz$$

$$\overset{\text{Eq.(D)}}{=} \frac{1}{\cancel{i\hbar}} \cancel{\frac{\hbar}{i}} \iiint_{-\infty}^{\infty} \psi^* \left(x \frac{\partial V}{\partial y} - y \frac{\partial V}{\partial x}\right)\psi \, dx\,dy\,dz$$

$$= -\iiint_{-\infty}^{\infty} \psi^* \left(x\frac{\partial V}{\partial y} - y\frac{\partial V}{\partial x} \right) \psi \, dx\,dy\,dz$$

$$= \langle \hat{D}_z \rangle .$$

The expression $\frac{d\langle \hat{L}_z \rangle}{dt} = \langle \hat{D}_z \rangle$

is an example of the Ehrenfest theorem.

In classical mechanics,

$$\frac{dL_z}{dt} = D_z \ , \text{ where}$$

$$D_z = (\vec{r} \times \vec{F})_z = xF_y - yF_x$$

$$= -\left(x\frac{\partial V}{\partial y} - y\frac{\partial V}{\partial x} \right) \text{ is a}$$

z-component of torque $\vec{D}$.

Thus, classically,

$$\frac{dL_z}{dt} = -\left(x\frac{\partial V}{\partial y} - y\frac{\partial V}{\partial x}\right). \quad (E)$$

In quantum mechanics, we replace observables by operators and then classical equations are preserved as long as we use expectation values instead of dynamical variables.

In our case, classical Eq. (E) becomes,

$$\frac{d\langle \hat{L}_z \rangle}{dt} = \left\langle -\left(\hat{x}\frac{\partial \hat{V}}{\partial y} - \hat{y}\frac{\partial \hat{V}}{\partial x}\right)\right\rangle$$

$$= \langle \hat{D}_z \rangle ,$$

where $\hat{D}_z$ is a quantum representation of D_z.

4. (a)

We know that

$$[\hat{x}, \hat{p}_x] = i\hbar \hat{1}, \text{ where}$$

$\hat{1}$ is a unit operator.

From the formula

$$[\hat{F}_1 \hat{F}_2, \hat{G}] = \hat{F}_1 [\hat{F}_2, \hat{G}] + [\hat{F}_1, \hat{G}] \hat{F}_2, \qquad (I)$$

we obtain,

$$[\hat{x}, \hat{p}_x^2] = -[\underset{\hat{F}_1}{\hat{p}_x}\underset{\hat{F}_2}{\hat{p}_x}, \underset{\hat{G}}{\hat{x}}] =$$

$$= -\left\{ \hat{p}_x[\hat{p}_x, \hat{x}] + [\hat{p}_x, \hat{x}]\hat{p}_x \right\}$$

$$= \hat{p}_x[\hat{x}, \hat{p}_x] + [\hat{x}, \hat{p}_x]\hat{p}_x =$$

$$= 2i\hbar\,\hat{p}_x .$$

$\therefore$

(b) $[\hat{x}^2, \hat{p}_x] \overset{Eq.(I)}{=} \hat{x}[\hat{x}, p_x] + [\hat{x}, \hat{p}_x]\hat{x} = 2i\hbar\hat{x}$.

(c) $[\hat{x}^2, \hat{p}_x^2] \overset{Eq.(I)}{=} \hat{x}[\hat{x}, \hat{p}_x^2] + [\hat{x}, \hat{p}_x^2]\hat{x} \overset{(a)}{=} \hat{x}(2i\hbar\hat{p}_x) + (2i\hbar\hat{p}_x)\hat{x} =$

$$= 2i\hbar(\hat{x}\hat{p}_x + \hat{p}_x x) .$$

An alternative form of $[\hat{x}^2, \hat{p}_x^2]$ can be obtained by using the fact that

$$\hat{x}\hat{p}_x - \hat{p}_x\hat{x} = i\hbar .$$

We obtain,

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

$$= 2i\hbar\left(2\hat{x}\hat{p}_x - i\hbar\right)$$

$$= 4i\hbar\,\hat{x}\hat{p}_x - 2(i\hbar)^2$$

$$= 4i\hbar\,\hat{x}\hat{p}_x + 2\hbar^2 ,$$

Finally,

$$[\hat{x}, \hat{H}] = [\hat{x}, \frac{\hat{p}_x^2}{2m} + \hat{V}] =$$

$$= \frac{1}{2m}[\hat{x}, \hat{p}_x^2] + [\hat{x}, \hat{V}] .$$

The latter commutator is zero, since

$$[\hat{x}, \hat{V}] = xV - Vx \text{ and}$$

V is a function of x only.

Thus,

$$[\hat{x},\hat{H}] = \frac{1}{2m}[\hat{x},\hat{p}_x^{\,2}] \overset{(a)}{=} \frac{1}{\cancel{2}m}\cancel{2}\,i\hbar\,\hat{p}_x = \frac{i\hbar}{m}\hat{p}_x .$$

Comment:

We are going to show in class that

$$\frac{d}{dt}\langle\hat{F}\rangle = \left\langle\frac{\partial\hat{F}}{\partial t}\right\rangle + \frac{1}{i\hbar}\langle[\hat{F},\hat{H}]\rangle,$$

where $\langle\,\rangle$ designates the expectation value.

For $\hat{F} = \hat{x}$, and $\hat{H} = \frac{\hat{p}_x^{\,2}}{2m} + \hat{V}(x)$

we obtain,

$$\frac{d}{dt}\langle\hat{x}\rangle = \Big\langle\underbrace{\frac{\partial\hat{x}}{\partial t}}_{=0}\Big\rangle + \frac{1}{i\hbar}\langle[\hat{x},\hat{H}]\rangle \underset{\text{above}}{\overset{\text{see}}{=}} \frac{1}{i\hbar}\,\frac{i\hbar}{m}\langle\hat{p}_x\rangle = \frac{1}{m}\langle\hat{p}_x\rangle.$$

Thus, $[\hat{x}, \hat{H}] = \frac{i\hbar}{m}\hat{p}_x$ <u>immediately</u> leads to the well-know Ehrenfest formula

$$\frac{d}{dt}\langle \hat{x} \rangle = \frac{1}{m}\langle \hat{p}_x \rangle .$$

Peter Breuer