4.1

(a.) $[x,y] = xy - yx = 0$

Same for $[x,z]$ and $[y,z]$, so $\boxed{[r_i, r_j]=0}$

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

$$= -\hbar^2\left(\frac{\partial^2 f}{\partial x\partial y} - \frac{\partial^2 f}{\partial y \partial x}\right) = 0$$ (Fubini's Thm on mixed partials)

$[p_x, p_z] = [p_y, p_z] = 0$ (similar reasoning), so $\boxed{[p_i,p_j]=0}$

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

so: $[x, p_x] = i\hbar$. Similarly, $[y, p_y] = [z, p_z] = i\hbar$

What about $[r_i, p_j]$ where $i \neq j$?

$$[y, p_x]f = -i\hbar\left[y\frac{\partial f}{\partial x} - \frac{\partial}{\partial x}(yf)\right] = -i\hbar\left[y\frac{\partial f}{\partial x} - y\frac{\partial f}{\partial x}\right] = 0$$

The same reasoning can be applied to all other commutation combos of $[r_i, p_j]$ where $i \neq j$.

$\therefore \quad [r_i, p_j] = i\hbar\delta_{ij}$

Last, if we switch the operators in the commutation relation when $i=j$:

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

$$= -i\hbar\left(x\frac{\partial f}{\partial x} + f - x\frac{\partial f}{\partial x}\right) = -i\hbar f$$

$[r_i, p_j] = -[p_i, r_j] = i\hbar\delta_{ij}$

(b.)

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

for all dimensions so we can just deal w/ x:

$$\frac{d\langle x\rangle}{dt} = \frac{i}{\hbar}\langle[\hat{H},\hat{x}]\rangle + \cancel{\left\langle\frac{\partial\hat{x}}{\partial t}\right\rangle} \rightarrow 0$$

no explicit dependence on time

$$\hat{H} = \frac{\hat{p}^2}{2m} + \hat{V} = \frac{\sum\hat{p}_i^2}{2m} + \hat{V}$$

$$\frac{d\langle x\rangle}{dt} = \frac{i}{\hbar}\left\langle\left[\frac{p_x^2+p_y^2+p_z^2}{2m} + V, x\right]\right\rangle$$

The only non-zero component of the RHS of this eqn is: $\frac{1}{2m}[p_x^2, x]$

Remember problem 3.13:

$$[\hat{A}\hat{B},\hat{C}] = \hat{A}[\hat{B},\hat{C}] + [\hat{A},\hat{C}]\hat{B}$$

$$\frac{1}{2m}[p_x^2, x] = \frac{1}{2m}\left\{p_x\underbrace{[p_x,x]}_{-i\hbar} + \underbrace{[p_x,x]}_{-i\hbar}p_x\right\}$$

$\leftarrow$ from $[p_i, r_j] = -i\hbar\delta_{ij}$

$$= \frac{\cancel{2}(-i\hbar)}{\cancel{2}m}p_x = \frac{-i\hbar}{m}p_x$$

$$\therefore \frac{d\langle x\rangle}{dt} = \frac{i}{\hbar}\left\langle\frac{-i\hbar}{m}p_x\right\rangle = \frac{1}{m}\langle p_x\rangle$$

Since the same argument can be used for x, y, and z, we have:

$$\frac{d\langle\bar{r}\rangle}{dt} = \frac{1}{m}\langle\bar{p}\rangle$$

QED

Now let's tackle $\frac{d\langle \vec{p} \rangle}{dt} = \langle -\nabla V \rangle$

Using the same logic as before; let's only deal w/ x:

$$\frac{d\langle p_x \rangle}{dt} = \frac{i}{\hbar}\langle [\hat{H}, p_x] \rangle$$

$$\hat{H} = \frac{p^2}{2m} + V$$

p_y^2 and p_z^2 commute w/ p_x so those terms are 0

$[p_x^2, p_x]$ also equals zero, since there's no distinction between $p_x^2 p_x$ and $p_x p_x^2$

$$\frac{d\langle p_x \rangle}{dt} = \frac{i}{\hbar}\langle [V, p_x] \rangle$$

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

$$= i\hbar f\frac{\partial V}{\partial x}$$

$$\frac{\partial\langle p_x \rangle}{dt} = \frac{i}{\hbar}(i\hbar)\left\langle \frac{\partial V}{\partial x} \right\rangle = -\left\langle \frac{\partial V}{\partial x} \right\rangle$$

Doing this same procedure for y and z gives:

$$\frac{d\langle \vec{p} \rangle}{dt} = -\left\langle \frac{\partial V}{\partial x} + \frac{\partial V}{\partial y} + \frac{\partial V}{\partial z} \right\rangle = -\langle \nabla V \rangle = \langle -\nabla V \rangle$$

QED

(c.) From Eqn. 3.62:

$$\sigma_A^2 \sigma_B^2 \geq \left(\frac{1}{2i}\langle [\hat{A}, \hat{B}] \rangle\right)^2$$

$\hat{A} = \hat{r}_i \quad \hat{B} = \hat{p}_j$

$$\sigma_A \sigma_B \geq \left|\frac{1}{2i}\langle [\hat{A}, \hat{B}] \rangle\right|$$

$$\sigma_{r_i}\sigma_{p_j} \geq \left|\frac{1}{2i}\langle [\hat{r}_i, \hat{p}_j] \rangle\right| = \left|\frac{1}{2i}\langle i\hbar\delta_{ij} \rangle\right| = \frac{\hbar}{2}\delta_{ij} \quad \text{QED}$$

← part (a.) →

4.2
$$V(x,y,z) = \begin{cases} 0 & x,y,z\ [0,a] \\ \infty & \text{otherwise} \end{cases}$$

$$\psi(x,y,z) = X(x)Y(y)Z(z)$$

$$-\frac{\hbar^2}{2m}\left(\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} + \frac{\partial^2\psi}{\partial z^2}\right) + 0\psi = E\psi$$

$$-\frac{\hbar^2}{2m}\left[YZ\frac{\partial^2 X}{\partial x^2} + XZ\frac{\partial^2 Y}{\partial y^2} + XY\frac{\partial^2 Z}{\partial z^2}\right] = E\psi$$

Divide by XYZ and isolate E

$$\underbrace{\frac{1}{X}\frac{\partial^2 X}{\partial x^2}}_{-k_x^2} + \underbrace{\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2}}_{-k_y^2} + \underbrace{\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2}}_{-k_z^2} = \frac{-2m}{\hbar^2}E$$

$$\frac{1}{X}\frac{\partial^2 X}{\partial x^2} = -k_x^2 \longrightarrow X(x) = A_x\sin(k_x x) + B_x\cos(k_x x)$$

$$\frac{1}{Y}\frac{\partial^2 Y}{\partial y^2} = -k_y^2 \longrightarrow Y(y) = A_y\sin(k_y y) + B_y\cos(k_y y)$$

$$\frac{1}{Z}\frac{\partial^2 Z}{\partial z^2} = -k_z^2 \longrightarrow Z(z) = A_z\sin(k_z z) + B_z\cos(k_z z)$$

$$-\frac{2m}{\hbar^2}E = -(k_x^2 + k_y^2 + k_z^2) \longrightarrow E = \frac{\hbar^2}{2m}(k_x^2 + k_y^2 + k_z^2)$$

Now let's use our BC's to eliminate terms:

$X(0) = 0$ so $B_x = 0$

$X(a) = 0$ so $k_x a = n\pi \longrightarrow k_x = \frac{n\pi}{a}$

Similarly, for Y and Z, we have $B_y = B_z = 0$ and $k_y = \frac{n_y\pi}{a}$ and $k_z = \frac{n_z\pi}{a}$

n_x, n_y, n_z can be any integer (not 0, though).
Negative values are redundant, so even though n_i can be negative, we only consider the positive values.

$$\therefore \quad \psi(x,y,z) = A_x A_y A_z \sin\left(\frac{n_x \pi}{a}\right) \sin\left(\frac{n_y \pi}{a}\right) \sin\left(\frac{n_z \pi}{a}\right)$$
$$\text{w/} \quad E = \frac{\hbar^2 \pi^2}{2ma^2}\left(n_x^2 + n_y^2 + n_z^2\right)$$

We can normalize each directional component separately:

$$1 = \underbrace{\int_0^a A_x^2 \sin^2\left(\frac{n_x \pi}{a}\right) dx}_{1} \underbrace{\int_0^a A_y^2 \sin^2\left(\frac{n_y \pi}{a}\right) dy}_{1} \underbrace{\int_0^a A_z^2 \sin^2\left(\frac{n_z \pi}{a}\right) dz}_{1}$$

$$1 = A_x^2 \int_0^a \frac{1 - \cos\left(\frac{2 n_x \pi}{a}\right)}{2} dx$$

$$= A_x^2 \left[\frac{a}{2} - \cancel{\frac{\sin(2 n_x \pi / a)\, a}{4 n_x \pi}\Bigg|_0^a}^{\to 0} \right]$$

$$\sqrt{\frac{2}{a}} = A_x \quad \rightarrow \quad A_y = A_z = \sqrt{\frac{2}{a}} \quad \text{(same reasoning)}$$

$$\boxed{\begin{aligned} \psi(x,y,z) &= \left(\frac{2}{a}\right)^{3/2} \sin\left(\frac{n_x \pi}{a}\right) \sin\left(\frac{n_y \pi}{a}\right) \sin\left(\frac{n_z \pi}{a}\right) \\ E &= \frac{\hbar^2 \pi^2}{2ma^2}\left(n_x^2 + n_y^2 + n_z^2\right) \quad \text{for } n_i = 1, 2, 3, \ldots \end{aligned}}$$

(b.)

	n_x	n_y	n_z	$\sum_i n_i^2$	Energy	Degeneracy
E_1	1	1	1	3	$3\frac{\hbar^2\pi^2}{2ma^2} = E_1$	1
E_2	2	1	1	6	$6\frac{\hbar^2\pi^2}{2ma^2} = 2E_1$	3
	1	2	1	6		
	1	1	2	6		
E_3	2	2	1	9	$9\frac{\hbar^2\pi^2}{2ma^2} = 3E_1$	3
	2	1	2			
	1	2	2			
E_4	1	1	3	11	$11\frac{\hbar^2\pi^2}{2ma^2} = \frac{11}{3}E_1$	3
	1	3	1			
	3	1	1			
E_5	2	2	2	12	$12\frac{\hbar^2\pi^2}{2ma^2} = 4E_1$	1
E_6	1	2	3	14	$14\frac{\hbar^2\pi^2}{2ma^2} = \frac{14}{3}E_1$	6
	1	3	2			
	2	1	3			
	2	3	1			
	3	1	2			
	3	2	1			

4.3 $\quad Y_0^0 = \sqrt{\frac{1}{4\pi}}$

$$Y_2^1 = -\left(\frac{15}{8\pi}\right)^{1/2} \sin\theta\cos\theta e^{i\phi}$$

$$P_\ell^m \equiv (1-x^2)^{|m|/2}\left(\frac{d}{dx}\right)^{|m|} P_\ell(x) \text{ , where } P_\ell(x) \equiv \frac{1}{2^\ell \ell!}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell$$

$$Y_\ell^m(\theta,\phi) = \epsilon\sqrt{\frac{(2\ell+1)}{4\pi}\frac{(\ell-|m|)!}{(\ell+|m|)!}} e^{im\phi} P_\ell^m(\cos\theta) \text{, where}$$

$\epsilon = (-1)^m$ for $m \geq 0$ and $\epsilon = 1$ for $m \leq 0$

$\ell = 0, m = 0$

$$Y_0^0(\theta,\phi) = (-1)^0\sqrt{\frac{1}{4\pi}\frac{0!}{0!}} e^0 P_0^0(\cos\theta)$$

$$P_0^0(\cos\theta) = \cancel{(1-\cos^2\theta)^0}^{\,1} \cancel{\left(\frac{d}{dx}\right)^0}^{\,1} P_0(\cos\theta)$$

$$P_0(\cos\theta) = \frac{1}{2^0 0!}\left(\frac{d}{dx}\right)^0(\cos^2\theta-1)^0 = 1$$

$$\boxed{Y_0^0(\theta,\phi) = \sqrt{\frac{1}{4\pi}}}$$

$$Y_2^1(\theta,\phi) = (-1)^1\sqrt{\frac{4+1}{4\pi}\frac{(1)!}{3!}} e^{i\phi} P_2^1(\cos\theta)$$

$$P_2^1(\cos\theta) = (1-\cos^2\theta)^{1/2}\frac{d}{d(\cos\theta)}\left[P_2(\cos\theta)\right] \qquad x = \cos\theta$$

$$P_2(\cos\theta) = \frac{1}{4\cdot 2!}\frac{d^2}{d(\cos\theta)^2}\left[(\cos^2-1)^2\right] \Rightarrow \frac{1}{8}\frac{d^2}{dx^2}\left[x^4-2x^2+1\right]$$

$$P_2(\cos\theta) = \frac{12}{8}x^2 - 4 = \frac{3}{2}\cos^2\theta - 1$$

$$P_2^1(\cos\theta) = (1-\cos^2\theta)^{1/2}\left[3\cos\theta\right] = 3\sin\theta\cos\theta$$

$$Y_2^1(\theta,\phi) = (-1)\sqrt{\frac{5}{4\pi\cdot 6}}\ 3\sin\theta\cos\theta\, e^{i\phi}$$

$$Y_2^1(\theta,\phi) = (-1)\sqrt{\frac{15}{8\pi}}\sin\theta\cos\theta\, e^{i\phi}$$

Normalization:

$$\int_0^{2\pi}\int_0^{\pi} |Y_0^0(\theta,\phi)|^2 \sin\theta\, d\theta\, d\phi = \frac{\cancel{2\pi}}{4\pi}\int_0^{\pi}\sin\theta\, d\theta = \frac{1}{2}\left[-\cos\theta\Big|_0^{\pi}\right]$$

$$= 1$$

$$\int_0^{2\pi}\int_0^{\pi} |Y_2^1(\theta,\phi)|^2 \sin\theta\, d\theta\, d\phi = \frac{15}{8\pi}\int_0^{\pi}\sin^2\theta\cos\theta\, d\theta\int_0^{2\pi} d\phi$$

$$= \frac{15\cdot\cancel{2\pi}}{4\,\cancel{8\pi}}\int_0^{\pi}\sin^3\theta\cos^2\theta\, d\theta = \frac{15}{4}\int_0^{\pi}\cos^2\theta(1-\cos^2\theta)\sin\theta\, d\theta$$

$x = \cos\theta$

$dx = -\sin\theta\, d\theta$

$$= \frac{-15}{4}\int_1^{-1} x^2(1-x^2)\,dx = \frac{15}{4}\int_{-1}^{1}(x^2-x^4)\,dx = \frac{15}{4}\left[\frac{x^3}{3}-\frac{x^5}{5}\right]_{-1}^{1}$$

$$= \frac{15}{4}\left[\frac{1}{3}-\frac{1}{5}-\left(\frac{-1}{3}\right)+\frac{(-1)^5}{5}\right] = \frac{15}{2}\left[\frac{5}{15}-\frac{3}{15}\right] = \frac{15}{2}\cdot\frac{2}{15} = 1$$

Orthogonality:

$x = \sin\theta$

$dx = \cos\theta\, d\theta$

$$\frac{1}{4\pi}\int_0^{2\pi}\int_0^{\pi}(-1)\sqrt{\frac{15}{2}}\sin\theta\cos\theta\, e^{i\phi}\, d\phi\, \sin\theta\, d\theta$$

$\sin\pi = 0$

$$-\sqrt{\frac{15}{2}}\frac{1}{4\pi}\int_0^{2\pi} e^{i\phi}\,d\phi\int_0^0 x^2\,dx = -\sqrt{\frac{15}{2}}\frac{1}{4\pi}\int_0^{2\pi} e^{i\phi}\,d\phi\left[\frac{x^3}{3}\Big|_0^0\right] = 0$$

$\sin 0 = 0$

4.6

$$\int_{-1}^{1} P_\ell(x) P_{\ell'}(x)\,dx \qquad P_\ell(x) \equiv \frac{1}{2^\ell \ell!}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell$$

$$\frac{1}{2^\ell \ell!}\frac{1}{2^{\ell'} \ell'!}\int_{-1}^{1}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell \left(\frac{d}{dx}\right)^{\ell'} (x^2-1)^{\ell'}\,dx$$

Case 1: $\ell > \ell'$

$$\frac{1}{(2^\ell \ell!)}\frac{1}{(2^{\ell'} \ell'!)}\int_{-1}^{1}\left(\frac{d}{dx}\right)^\ell (x^2-1)^\ell \left(\frac{d}{dx}\right)^{\ell'} (x^2-1)^{\ell'}\,dx$$

IBP

$$\frac{1}{(2^\ell \ell!)}\frac{1}{(2^{\ell'} \ell'!)}\left\{\underbrace{\left[\left(\frac{d}{dx}\right)^{\ell-1}(x^2-1)^\ell\right]\left[\left(\frac{d}{dx}\right)^{\ell'}(x^2-1)^{\ell'}\right]\Bigg|_{-1}^{1}}_{\text{Boundary term}} - \int_{-1}^{1}\left[\left(\frac{d}{dx}\right)^{\ell-1}(x^2-1)^\ell\right]\left[\left(\frac{d}{dx}\right)^{\ell'+1}(x^2-1)^{\ell'}\right]dx\right\}$$

If we IBP successively, (always targeting the ℓ term since $\ell > \ell'$), then we get the following after ℓ IBPs:

$$\text{Boundary terms} + (-1)^\ell \int_{-1}^{1}(x^2-1)\left(\frac{d}{dx}\right)^{\ell'+\ell}(x^2-1)^{\ell'}\,dx$$

Since $\ell'+\ell > 2\ell$, taking the x derivative $\ell'+\ell$ times of $(x^2-1)^{\ell'}$ (whose largest term is $x^{2\ell'}$) will give 0.

Now let's look @ the boundary terms, which look like this

$$\sum \left[\left(\frac{d}{dx}\right)^{\ell-n}(x^2-1)^\ell\right]\left[\left(\frac{d}{dx}\right)^{\ell'+n-1}(x^2-1)^{\ell'}\right]\Bigg|_{-1}^{+1} \quad \text{where } n = 1, 2, 3, \ldots \ell$$

For each term, $l-n = 0, 1, 2, \dots$ or $l-1$, so the $\left(\frac{d}{dx}\right)^{l-n}$ derivative of $(x^2-1)^l$ will always leave an overall (x^2-1) term. Since $(x^2-1)\Big|_{-1}^{1} = 0$, each boundary term is 0.

$$\therefore \int_{-1}^{1} P_l(x) P_{l'}(x)\, dx = 0$$

Case 2: $l = l'$

$$\left(\frac{1}{2^l l!}\right)^2 \int_{-1}^{1} [P_l(x)]^2 dx = \left(\frac{1}{2^l l!}\right)^{2} \int_{-1}^{1} \left[\left(\frac{d}{dx}\right)^l (x^2-1)^l\right]^2 dx$$

IBP l times gives:

$$= \text{Boundary terms} + \frac{(-1)^l}{(2^l l!)^2} \int_{-1}^{1} (x^2-1)^l \left(\frac{d}{dx}\right)^{2l} (x^2-1)^l dx$$

As before, the boundary terms go to 0. Differentiating x^{2l} (from $[x^2-1]^l$) $2l$ times (all other terms go to 0):

$$= \frac{(-1)^l (2l)!}{(2^l l!)^2} \int_{-1}^{1} (x^2-1)^l dx = \frac{(2l)!}{(2^l l!)^2} \int_{-1}^{1} (1-x^2)^l dx$$

$$= \frac{(2l)!}{(2^l l!)^2} \int_{-1}^{1} (1-x^2)^l dx$$

Let's do a substitution here: $x = 2u - 1$; $dx = 2du$

$$= \frac{2(2l)!}{(2^l l!)^2} \int_{0}^{1} \left(1 - [2u-1]^2\right)^l du = \frac{2(2l)!}{(2^l l!)^2} \int_{0}^{1} [1-4u^2+4u-1]^l du$$

$1 - 4u^2 + 4u - 1$

$$= \frac{2(2\ell)!}{(2^\ell \ell!)^2}\int_0^1 2^{2\ell}[u-u^2]^\ell du = \frac{2(2\ell)!}{(2^\ell \ell!)^2} 2^{2\ell}\int_0^1 u^\ell (1-u)^\ell du$$

The Beta function, $B(r,s)$, can be defined as:

$$B(r,s) = \int_0^1 x^{r-1}(1-x)^{s-1}dx = \frac{\Gamma(r)\Gamma(s)}{\Gamma(r+s)}$$

$$B(\ell+1,\ell+1) = \int_0^1 x^\ell(1-x)^\ell dx$$

$$= \frac{2(2\ell)!}{\cancel{2^{2\ell}}(\ell!)^2}\cancel{2^{2\ell}} \frac{\Gamma(\ell+1)\Gamma(\ell+1)}{\Gamma(\ell+1+\ell+1)} = \frac{2(2\ell)!}{(\ell!)^2}\frac{[\Gamma(\ell+1)]^2}{\Gamma(2\ell+2)}$$

$\Gamma(\ell+1) = \ell!$

$\Gamma(2\ell+2) = (2\ell+1)!$

$$= \frac{2(2\ell)!}{\cancel{(\ell!)^2}}\frac{\cancel{(\ell!)^2}}{(2\ell+1)!} = \frac{2\cancel{(2\ell)!}}{(2\ell+1)\cancel{(2\ell)!}} = \frac{2}{2\ell+1}$$

Since only the $\ell=\ell'$ case is non-zero, we have

$$\boxed{\int_{-1}^1 P_\ell(x)P_{\ell'}(x)dx = \frac{2}{2\ell+1}\delta_{\ell\ell'} \qquad \text{QED}}$$