Assignment 3.

① $\hat{H}_{el} = -\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{\hbar^2}{2m}\nabla_3^2 + V(x_1) + V(x_2) + V(x_3) + \frac{e^2}{4\pi\varepsilon_0|x_1-x_2|} + \frac{e^2}{4\pi\varepsilon_0|x_2-x_3|} + \frac{e^2}{4\pi\varepsilon_0|x_1-x_3|}$

$$\underbrace{-\frac{\hbar^2}{2m}\nabla_1^2 - \frac{\hbar^2}{2m}\nabla_2^2 - \frac{\hbar^2}{2m}\nabla_3^2}_{\text{kinetic energy of 3 } e^-} + \underbrace{V(x_1) + V(x_2) + V(x_3)}_{\text{external potential}} + \underbrace{\frac{e^2}{4\pi\varepsilon_0|x_1-x_2|} + \frac{e^2}{4\pi\varepsilon_0|x_2-x_3|} + \frac{e^2}{4\pi\varepsilon_0|x_1-x_3|}}_{e^--e^-\text{ repulsions, internal potential.}}$$

② $\Psi_{n_x,n_y}(x,y) = \left(\frac{4}{ab}\right)^{1/2}\sin\left(\frac{n_x\pi x}{a}\right)\sin\left(\frac{n_y\pi y}{b}\right)$

a) $\int_0^a\int_0^b \Psi^*_{n_x,n_y}\Psi_{n_x,n_y}\,dx\,dy = \int_0^a dx\int_0^b dy\left(\frac{4}{ab}\right)\sin^2\left(\frac{n_x\pi x}{a}\right)\sin^2\left(\frac{n_y\pi y}{b}\right)$

$= \left(\frac{4}{ab}\right)\underbrace{\left[\int_0^a dx\sin^2\left(\frac{n_x\pi x}{a}\right)\right]\left[\int_0^b dy\sin^2\left(\frac{n_y\pi y}{b}\right)\right]}_{\text{same integrals}}$

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

$= \frac{1}{2}\left\{x - \left[\sin\left(\frac{2n_x\pi x}{a}\right)\right]\left[\frac{a}{2n_x\pi}\right]\right\}\Big|_0^a$

$= \frac{a}{2} - 0 - 0 - 0 = \frac{a}{2}$.

$= \left(\frac{4}{ab}\right)\left(\frac{a}{2}\right)\left(\frac{b}{2}\right) = 1$, normalized.

b) $\int_0^{a/2}dx\int_0^{b/2}dy\left(\frac{4}{ab}\right)\left(\frac{1}{2}\left[1-\cos\left(\frac{n_x\pi x}{a}\right)\right]\right)\left(\frac{1}{2}\left[1-\cos\left(\frac{n_y\pi y}{b}\right)\right]\right) = \left(\frac{4}{ab}\right)\left(\frac{1}{4}\right)\int_0^{a/2}dx\left(1-\cos\left(\frac{n_x\pi x}{a}\right)\right)\int_0^{b/2}dy\left(1-\cos\left(\frac{n_y\pi y}{b}\right)\right)$

$= \left(\frac{1}{ab}\right)\left(\frac{a}{2}\right)\left(\frac{b}{2}\right) = \frac{1}{4} = 0.25$.

c) Yes, because of symmetry.

d) $E = \frac{h^2}{8m}\left[\left(\frac{n_x}{a}\right)^2 + \left(\frac{n_y}{b}\right)^2\right]$

	n_x	n_y	$E(\times h^2/8m)$
G.S	1	1	$\frac{1}{a^2}+\frac{1}{b^2}$
possible lowest energy excited states	1	2	$\frac{1}{a^2}+\frac{4}{b^2}$
	2	1	$\frac{4}{a^2}+\frac{1}{b^2}$

$\underbrace{\frac{1}{a^2}+\frac{4}{b^2} = \frac{1}{b^2}+\frac{4}{a^2}}$

→ must satisfy this to be degenerate

→ $a = b$

$\frac{1}{a^2}+\frac{4}{a^2} = \frac{1}{a^2}+\frac{4}{a^2} = \frac{5}{a^2}$.

③ $a = 5Å$

n_x	n_y	n_z	$E(\times \frac{h^2}{8ma^2})$
1	1	1	2.01
2	1	1	5.01
1	2	1	5.01
1	1	2	2.02
1	1	10	3.00

n_x	$E(\times \frac{h^2}{8ma^2})$
1	0.01
2	0.02
10	1.00

n_i: x	y	z	n_f: x	y	z	λ (m)
1	1	1	2	1	1	2.75×10^{-7} m
1	1	1	1	2	1	2.75×10^{-7}
1	1	1	1	1	2	8.24×10^{-5}
1	1	1	1	1	10	8.32×10^{-7}

n_i	n_f	λ (m)
1	2	8.24×10^{-5}
1	10	8.32×10^{-7}

just a sample of possible values one can try.

transitions are similar so spectrum is similar

④ $\Psi_4(x) = \sqrt{\frac{2}{a}}\sin\left(\frac{4\pi x}{a}\right) = 0$

$\sin\left(\frac{4\pi x}{a}\right) = 0$

$x = \left\{0, \boxed{\frac{a}{4}, \frac{a}{2}, \frac{3a}{4}}, a\right\}$

3 nodes.

⑤ $\hat{A}$ and $\hat{B}$ commute if $[\hat{A},\hat{B}]\Psi(x,y,z) = \hat{A}\hat{B}\Psi(x,y,z) - \hat{B}\hat{A}\Psi(x,y,z)$

$[\underbrace{-i\hbar\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)}_{\hat{l}_x}, \underbrace{-i\hbar\left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right)}_{\hat{l}_y}]\Psi = (i\hbar)^2\left[\left(y\frac{\partial}{\partial z}-z\frac{\partial}{\partial y}\right)\left(z\frac{\partial\Psi}{\partial x}-x\frac{\partial\Psi}{\partial z}\right) - \left(z\frac{\partial}{\partial x}-x\frac{\partial}{\partial z}\right)\left(y\frac{\partial\Psi}{\partial z}-z\frac{\partial\Psi}{\partial y}\right)\right]$

$= -\hbar^2\left[y\left(\frac{\partial\Psi}{\partial x} + z\frac{\partial^2\Psi}{\partial z\partial x} - 0 - x\frac{\partial^2\Psi}{\partial z^2}\right) - z\left(0 + z\frac{\partial^2\Psi}{\partial y\partial x} - 0 - x\frac{\partial^2\Psi}{\partial y\partial z}\right)\right.$
$\left. - z\left(0 + y\frac{\partial^2\Psi}{\partial x\partial z} - 0 - z\frac{\partial^2\Psi}{\partial x\partial y}\right) + x\left(0 + y\frac{\partial^2\Psi}{\partial z^2} - \frac{\partial\Psi}{\partial y} - z\frac{\partial^2\Psi}{\partial z\partial y}\right)\right]$

$= -\hbar^2\left[y\frac{\partial\Psi}{\partial x} + \boxed{yz\frac{\partial^2\Psi}{\partial x\partial z}} - xy\frac{\partial^2\Psi}{\partial z^2} - z^2\frac{\partial^2\Psi}{\partial x\partial y} + xz\frac{\partial^2\Psi}{\partial y\partial z} - \boxed{yz\frac{\partial^2\Psi}{\partial x\partial z}} + z^2\frac{\partial^2\Psi}{\partial x\partial y}\right.$
$\left. + xy\frac{\partial^2\Psi}{\partial z^2} - x\frac{\partial\Psi}{\partial y} - xz\frac{\partial^2\Psi}{\partial y\partial z}\right]$

$= -\hbar^2\left[y\frac{\partial\Psi}{\partial x} - x\frac{\partial\Psi}{\partial y}\right] = -\hbar^2\underbrace{\left[y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right]}_{\hat{l}_z}\Psi$

$= -\hbar^2\hat{l}_z\Psi$

$\hat{l}_x$ and $\hat{l}_y$ don't commute.