1) For an electron confined to a 2-dimensional box of length 0.1 nm, what is the kinetic energy of the ground state? How does this compare to the energy of an electron confined to a 1-dimensional box?

From lecture notes: \( E_{nx,ny} = -\frac{\hbar^2 \pi^2}{2mL^2} (n_x^2 + n_y^2) \), ground state \( n_x = 1, n_y = 1 \)

\[ L = 0.1 \text{ nm}, m = 0.511 \text{ MeV}/c^2, \ (\hbar c)^2 = (197.33 \text{ eV}*\text{nm})^2 \]

\[ E_{nx,ny} = -\frac{(\hbar c)^2 \pi^2}{2mc^2L^2} (n_x^2 + n_y^2)^*2 = (37.6 \text{ eV})^2 = 75.2 \text{ eV} \]

The one dimensional solution is \( E_n = n^2 \frac{\hbar^2 \pi^2}{2mc^2L^2} = 37.6n^2 \text{ eV} \)

2) An electron is trapped in an infinite square-well potential of width 0.5 nm. If the electron is initially in the \( n=4 \) state, what are the various photon energies that can be emitted as the electron jumps to the ground state? (T&R problem 6-21)

\[ L = 0.5 \text{ nm}, m = 0.511 \text{ MeV}/c^2, \ (\hbar c)^2 = (197.33 \text{ eV}*\text{nm})^2 \]

\[ E_1 = \frac{(\hbar c)^2 \pi^2}{2mc^2L^2} = 1.504 \text{ eV}, \ E_n = n^2E_1 \]

\[ E_{4-3} = (4^2 - 3^2)E_1 = 10.53 \text{ eV} \]
\[ E_{4-2} = (4^2 - 2^2)E_1 = 18.05 \text{ eV} \]
\[ E_{4-1} = (4^2 - 1^2)E_1 = 22.56 \text{ eV} \]
\[ E_{3-2} = (3^2 - 2^2)E_1 = 7.52 \text{ eV} \]
\[ E_{3-1} = (3^2 - 1^2)E_1 = 12.03 \text{ eV} \]
\[ E_{2-1} = (2^2 - 1^2)E_1 = 4.51 \text{ eV} \]
3) How many different energy levels can a particle in a 2-dimensional box have that are less than 60E₀ where \( E₀ = \frac{\pi^2 \hbar^2}{2mL^2} \)? Show your work.

\[(n_x^2 + n_y^2)E₀ < 60E₀\]  
Note: No preferred direction  \( \therefore \) energy levels are symmetric for \( x, y \) values: \( E(3,1) = E(1,3) \) (degeneracy)

Start by finding max \( n_x \): \( n_x = (60 - 1)^{1/2} = (59)^{1/2} < 8 \) so \( n_x = 7 \)
\( E(7,1) \rightarrow 50E₀, E(7,2) \rightarrow 53E₀, E(7,3) \rightarrow 58E₀ \) this is the max

Now find the \( n_x = n_y \) max, \( 2n^2 = 60 \rightarrow n = (30)^{1/2} < 6 \) so \( n = 5 \)
\( n_y \) will never exceed 5 for \( n_x \rightarrow E(7,1) \) (Any that exceed 5 are repeats or yield more than 60E₀)

\[
\begin{array}{ccccccc}
5 & 4 & 3 & 2 & 1 \\
7 & 74 & 65 & 58 & 53 & 50 \\
6 & 61 & 52 & 45 & 40 & 37 \\
5 & 50 & 41 & 34 & 29 & 26 \\
4 & 41 & 32 & 25 & 20 & 17 \\
3 & 34 & 25 & 18 & 13 & 10 \\
2 & 29 & 20 & 13 & 8 & 5 \\
1 & 26 & 17 & 10 & 5 & 2 \\
\end{array}
\]

Color code:

*blue numbers are the possible energy levels
*black numbers represent combinations that do not meet criteria
*red numbers are degenerate solutions (repeats)
*green numbers are the combinations that are left over

Note: \( E(7,1) \) and \( E(5,5) \) represent special degeneracy

So there are 21 allowable states (22 if counting \( E(7,1) \) and \( E(5,5) \) as different energy states)
4) The harmonic oscillator potential is \( U(x) = (1/2)m\omega_0^2x^2 \); a particle of mass \( m \) in this potential oscillates with frequency \( \omega_0 \). The ground-state wavefunction for a particle in the harmonic oscillator potential has the form \( \psi(x) = A \exp(-ax^2) \).

By substituting \( U(x) \) and \( \psi(x) \) into the one-dimensional time-independent Schrödinger Equation, find expressions for the ground-state energy \( E \) and the constant \( a \) in terms of \( m \), \( \hbar \), and \( \omega_0 \).

Start with the time independent Schrödinger Equation

\[
-\frac{\hbar^2}{2m} \frac{d^2 \psi(x)}{dx^2} + U(x)\psi(x) = E\psi(x) \quad \psi(x) = A \exp(-ax^2) \quad \Rightarrow \quad \mathcal{E}(x) = \frac{1}{2}m\omega_0^2 \psi^2
\]

To use the time independent Schrödinger Equation, a wavefunction must be determined. So a normalization constant is needed.

\[
\int_{-\infty}^{\infty} A^2 e^{-2ax^2} \, dx = 1 \Rightarrow A^2 \sqrt{\frac{\pi}{2a}} = 1 \rightarrow A = \left( \frac{2a}{\pi} \right)^{1/4}
\]

Next take the first and second derivatives of the wave function

\[
\frac{d}{dx} \psi(x) = -2x \quad a \quad \Rightarrow \quad \frac{d}{dx} \psi(x) = -2ax A \exp(-ax^2)
\]

\[
\frac{d}{dx} \left( \frac{d}{dx} \psi(x) \right) = 4A^2 e^{-2ax^2} x^2 - 2a \quad \Rightarrow \quad \frac{d}{dx} \left( \frac{d}{dx} \psi(x) \right) = -2a \frac{d}{dx} \psi(x)
\]

Sub parts into the time independent Schrödinger Equation and do some algebra

\[
A e^{-ax^2} \left[ \frac{-\hbar^2}{2m} \left( \frac{2a}{m} \right)^2 x^2 - a + \frac{1}{2} m\omega_0^2 x^2 - E \right] = 0
\]

Then do some more algebra

\[
x^2 \left( -\frac{2\hbar^2}{m} a^2 + \frac{1}{2} m\omega_0^2 \right) - \left( E - \frac{\hbar^2 a}{m} \right) = 0
\]

The quantities in parenthesis are both equal to zero, so

\[-2\hbar^2 a^2/m = -m\omega_0^2/2 \rightarrow a = m\omega_0/\hbar
\]

And

\[E = \hbar^2 a/m = (\hbar^2/m)*(m\omega_0/2 \hbar) = (1/2) \hbar \omega_0
\]
5) The H2 molecule can be approximated by a simple harmonic oscillator having spring constant $k=1.1 \times 10^3 \text{ N/m}$. Find (a) the energy levels and (b) the possible wavelengths of photons emitted with the H2 molecule decays from the third excited state eventually to the ground state.

(a) We simplify H2 as a harmonic oscillator, so the reduced mass is $\frac{m \text{m}}{m + m} = \frac{m}{2}$ and the spring constant $k=1100 \text{ N/m}$. Thus the energies are $E_n=(n+1/2)\hbar \omega$, where $\omega=\sqrt{\frac{2k}{m}}$ and $m$ is the mass of H atom. And $\hbar \omega=0.759 \text{ ev}=1.214 \times 10^{-19} \text{ J}$

(b) Ground state $E_0=1/2 \hbar \omega$, and the third excited state $E_3=(3+1/2)\hbar \omega$.

So $\Delta E=E_3-E_0=3 \hbar \omega = 3 \hbar \sqrt{2 \frac{k}{m}} = 3.644 \times 10^{-19} \text{ J}=2.278 \text{ ev}$.

$$\lambda = \frac{hc}{\Delta E} = 545.8 \text{ nm}.$$
6) Calculate the probability that an electron in the ground state of the hydrogen atom can be found between 0.95\(a_0\) and 1.05\(a_0\).

The ground state for the hydrogen atom is \(n = 0, l = 0, m_s = 0\)

\[
\Psi(r) \rightarrow R_{nl}(r) = \frac{2}{a_0^{3/2}} e^{-r/a_0}
\]

And

\[
P_{nl}(r) = r^2 \cdot \left( \frac{2}{a_0^{3/2}} \right)^2 e^{-2r/a_0}
\]

So the probability is

\[
\frac{4}{a_0^3} \int_{0.95a_0}^{1.05a_0} r^2 e^{-2r/a_0} \, dr = 5.41\%
\]

7) The 3-D Schrödinger Equation (S.E.) for the hydrogen atom looks like:

\[
\frac{-\hbar^2}{2m} \left[ \frac{\partial^2 \psi}{\partial r^2} + \frac{2}{r} \frac{\partial \psi}{\partial r} + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left( \sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \psi}{\partial \phi^2} \right] + U(r)\psi = E\psi
\]

where

\[
U(r) = -\frac{1}{4\pi \varepsilon_0} \frac{e}{r}
\]

show that \(\psi(r, \theta, \phi) = \frac{1}{\sqrt{\pi a_0^{3/2}}} e^{-r/a_0}\) satisfies this equation provided

\[
E = -\frac{me^4}{32\pi^2 \varepsilon_0^2 \hbar^2} \quad \text{(ground state energy of the H atom)}
\]

and \(a_0\) (Bohr radius)
Take derivatives:  (a) \( \frac{\partial \psi}{\partial r} = -e^{-r/a_0} \sqrt{\pi a_0^{3/2}} \), (b) \( \frac{\partial^2 \psi}{\partial r^2} = \frac{e^{-r/a_0}}{\sqrt{\pi a_0^{7/2}}} \), (c) \( \frac{\partial \psi}{\partial \theta} = \frac{\partial \psi}{\partial \phi} = 0 \)

plug (a) (b) (c) into the time independent S.E.

\(-\frac{\hbar^2}{2m} \left[ \frac{\partial^2 \psi}{\partial r^2} + \frac{2r}{m} \frac{\partial \psi}{\partial r} + 0 + 0 \right] + U(r) \psi(r) = E^* \psi(r)\)

\[
\left( -\frac{\hbar^2}{2m} \cdot \frac{e^{-r/a_0}}{\sqrt{\pi a_0^{7/2}}} \right) + \left( -\frac{\hbar^2}{2mr} \cdot \frac{e^{-r/a_0}}{\sqrt{\pi a_0^{5/2}}} \right) - \left( \frac{e^2}{4\pi \varepsilon_0 r} \cdot \frac{e^{-r/a_0}}{\sqrt{\pi a_0^{3/2}}} \right) = E \cdot \frac{e^{-r/a_0}}{\sqrt{\pi a_0^{3/2}}}
\]

\[
\left( -\frac{\hbar^2}{2m} \cdot \frac{1}{a_0^2} \right) + \left( -\frac{\hbar^2}{2mr} \cdot \frac{1}{a_0} \right) - \left( \frac{e^2}{4\pi \varepsilon_0 r} \right) = E
\]

\[
\left( -\frac{\hbar^2}{2m} \cdot \frac{1}{a_0^2} \right) - E + \frac{1}{r} \left[ \left( -\frac{\hbar^2}{2m} \cdot \frac{1}{a_0} \right) - \left( \frac{e^2}{4\pi \varepsilon_0} \right) \right] = 0
\]

For this to be true for all \( r \),

\[
\left( -\frac{\hbar^2}{2m} \cdot \frac{1}{a_0^2} \right) = \left( \frac{e^2}{4\pi \varepsilon_0} \right)
\]

(solve for \( a_0 \)) \( a_0 = (4\pi \varepsilon_0 \hbar^2)/me^2 \)

Also...

\[
\left( \frac{\hbar^2}{2m} \cdot \frac{1}{a_0^2} \right) = E
\]

Plug in \( a_0 \) to find \( E \) using above equation to get

\[
E = \frac{1}{a_0} \cdot e^2/8\pi \varepsilon_0 \quad \text{and} \quad E = \frac{me^4}{32\pi^2 \varepsilon_0^2 \hbar^2}
\]

**Extra Credit:**

\( E = 65E_0, 85E_0, 125E_0 \)

Need to attach your calculations or your computer program.