1. (Use *Mathematica*)
   According to the LCAO-MO theory of the electronic structure of molecules, the wavefunctions of a molecule ("molecular orbitals") are described by a linear combination of atomic orbitals. The number of molecular orbitals (MOs) is equal to the number of atomic orbitals used to construct them. The H_2^+ ion is a simple example of the application of LCAO-MO theory. Two 1s orbitals, one from each H atom, can be added and subtracted to form the bonding and antibonding MOs, respectively, with σ symmetry (cylindrically symmetric about bond axis). Using x and y to define coordinates (in units of a_0, the Bohr radius) relative to one of the two H atoms in a plane perpendicular to the bond axis, the bonding and antibonding MOs, σ_{1s} and σ_{1s}^*, may be written as:

$$\sigma_{1s}(x,y) = e^{-(x^2+y^2)/2} + e^{-[(x-d)^2+y^2]/2}$$

$$\sigma_{1s}^*(x,y) = e^{-(x^2+y^2)/2} - e^{-[(x-d)^2+y^2]/2}$$

   where *d* is the equilibrium bond length (in units of a_0), which is equal to 2.5 in this problem.

   As you do the following, please note the differences between the bonding and antibonding orbitals (most notably, the constructive interference between the 1s orbital that leads to enhanced amplitude and electron probability in the bonding orbital, and the node at the middle of the bond in the antibonding orbital).

   (a) Use **Plot3D** to plot , σ_{1s} and σ_{1s}^* over the ranges $-4 \le x \le 6$ and $-3 \le y \le 3$. Include the **PlotRange → All** option to force all your surface to be displayed.

   (b) Make contour plots of the probability densities, $(\sigma_{1s})^2$ and $(\sigma_{1s}^*)^2$, over the ranges $-2 \le x \le 4.5$ and $-2.5 \le y \le 2.5$.

   (c) Make density plots of the probability densities, $(\sigma_{1s})^2$ and $(\sigma_{1s}^*)^2$, over the ranges $-2 \le x \le 4.5$ and $-2.5 \le y \le 2.5$, in **GrayTones**.

2. *(Use Mathematica)*
   In Cartesian coordinates (atomic units), the $4f_{z^2}$ orbital of the hydrogen atom is proportional to the following function:

$$f(x,y,z) = z(3x^2 + 3y^2 - 2z^2)e^{-r/4}$$

   where $r = (x^2 + y^2 + z^2)^{1/2}$.

   (a) Use **ContourPlot3D** to plot three-dimensional surfaces of the *f(x,y,z)*=0.2 and *f(x,y,z)*=-0.2 contours. Choose ranges of *x*, *y*, and *z* such that the surfaces are not cut off. Label your axes and use different colors to display the positive and negative contour surfaces.

(b) Use **ContourPlot** to make a contour plot of the projection of *f(x,y,z)* in the yz-plane (i.e., x=0) with $-40 \leq y \leq 40$ and $-40 \leq z \leq 40$. Label your axes, use 20 contour levels in your plot, and use **PlotRange** $\rightarrow$ **All** to display the full range of the function.

(c) Use **DensityPlot** to plot the projection of $r^2[f(x,y,z)]^2$, which is proportional to the electron probability density, in the yz-plane with $-40 \leq y \leq 40$ and $-40 \leq z \leq 40$. Label your axes and use use **PlotRange** $\rightarrow$ **All** to display the full range of the function.