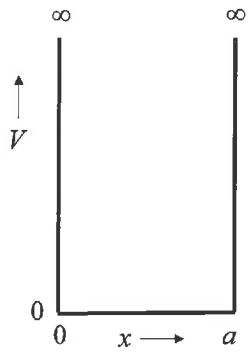
Interim exam 6A7X2 part Advanced Chemical Bonding
Tuesday February 26 2019, 17.30-19.30 h

It is allowed to use a (graphing) calculator

Problem 1 (25 points)
We consider the wave function $\psi(x) = N \cdot x(a-x)$ that describes a particle in a box with width a and infinite walls as shown schematically below. The potential energy in the box is zero: $V(x) = 0$ for $0 \leq x \leq a$, outside the box the potential is infinite: $V(x) = \infty$, for $x < 0$ and $x > a$.



a. (5 pt) Normalize the wave function.

b. (10 pt) Calculate the expectation values $\langle x^2 \rangle$ and $\langle p_x^2 \rangle$.

c. (5 pt) What is the energy associated with this wave function?

d. (5 pt) Show that the Heisenberg relation $\hat{x}\hat{p}_x - \hat{p}_x\hat{x} = i\hbar$ holds.

Problem 2 (20 points)

BH_3 has a three-fold symmetry, meaning that three hydrogen atoms have identical properties. Two molecular orbitals of BH_3 can be formed by taking a linear combination of the boron $2s$ orbital and an orbital ϕ that is linear combination of the three $1s$ orbitals of the thee hydrogen atoms A, B and C. ϕ is given by:

$$\phi = 1s_A + 1s_B + 1s_C$$

Further the following integrals are given (in unspecified units for the integrals in the right column):

$$\langle 2s|2s\rangle = 1 \qquad \left\langle 2s\left|\hat{F}\right|2s\right\rangle = -6.000$$

$$\langle 1s_A|1s_A\rangle = 1 \qquad \left\langle 1s_A\left|\hat{F}\right|1s_A\right\rangle = -3.000$$

$$\langle 1s_A|2s\rangle = 0 \qquad \left\langle 1s_A\left|\hat{F}\right|2s\right\rangle = -1.155$$

$$\langle 1s_A|1s_B\rangle = 0 \qquad \left\langle 1s_A\left|\hat{F}\right|1s_B\right\rangle = 0.000$$

The integrals that are not specified above follow directly from the symmetry of the molecule. We will determine the energies of the two molecular orbitals of BH_3 formed in the basis of the two functions $2s$ and ϕ.

a. (5 pt) Determine the values for the overlap integrals $\langle\phi|\phi\rangle$ and $\langle\phi|2s\rangle$.

b. (5 pt) Determine the values for the Fock integrals $\left\langle\phi\left|\hat{F}\right|\phi\right\rangle$ and $\left\langle\phi\left|\hat{F}\right|2s\right\rangle$.

c. (5 pt) Determine the overlap matrix **S** and the Fock matrix **F** in the $2s$ and ϕ basis.

d. (5 pt) Set up the Roothaan equation for the molecular orbitals that are linear combinations of $2s$ and ϕ. Determine the molecular orbital energies from the secular equation.