3.012 PS 2 **3.012**
Issued: 09.20.05 **Fall 05**
Due: 09.30.05

No plagiarism allowed: see the handbook for students at http://web.mit.edu/due/handbook.pdf . On the other hand, you should feel free to consult as much as possible books and other educational material. Remember that the homework is primarily designed to give you a chance to gauge your understanding of the material – if you struggle with a concept, go back to the lecture notes, the textbook, the TAs, the instructor.

BONDING

1. Determine which of the following operators are linear:

   a. $\hat{O}$, defined as $\hat{O}(f) = \frac{d^2 f}{dx^2}$

   b. $\hat{O}$, defined as $\hat{O}(f) = \left(\frac{df}{dx}\right)^2$

2. Calculate the commutator between $\hat{x}$ and $\hat{p}_x$, and that between $\hat{x}$ and $\hat{p}_y$.

3. What is the potential felt by an electron in the presence of the nucleus of a helium atom ? Draw it as a function of the radial distance from the nucleus. When that electron is in a bound state (i.e. we have He^+), what will be its energy levels ? Now, suppose we had the second electron approach this positive ion He^+ . Can you draw the potential that the second electron feels when it is very distant from He^+ ? Can you say what its analytic form will be ?

4. Use Appendix A.4.2 (the one on Spherical Coordinates – my textbook might have a different numbering than yours) to calculate the volume of the skin of a Valencia orange. Assume that the outer radius of the orange is .05 m, and the thickness of the skin .005 m.

5. What is the expectation value for the potential energy of an electron in the 2s state of the hydrogen atom ? Derive explicitly and explain all the steps in obtaining your result (use paragraph 20.3 in your textbook to obtain the wavefunctions). How does this result compares with the one for the total energy given in formula 20.7 ? Can you then derive the expectation value for the kinetic energy, without explicitly performing the needed derivatives and integrals ?

6. Show that the 1s and 2s wavefunctions of the electron in the hydrogen atom are orthogonal: $\langle \psi_{1s} | \psi_{2s} \rangle = 0$. As a side note, it is this constraint of orthonormality that forces the 2s electrons in an atom to be, on average, further away from the nucleus than the 1s electrons.

7. Sketch the radial part and the angular part of all 3d wavefunctions for the hydrogen atom, and describe the nodal surfaces (i.e. where it goes to zero).

8. If the wavefunction for an electron in a central potential has a principal quantum number n=3 and angular momentum quantum number l=1, what wi ll be the possible values for the magnetic quantum number m ? How many nodes will characterize the radial wavefunction for the above electron ?

9. What is the Aufbau principle ? Is it an absolute law of nature?

THERMODYNAMICS

10. A sheet of manganese (2 moles) at room temperature (298 K) is placed in thermal contact with a heat supply that slowly transfers 100,698 J of heat into the sample at constant pressure. Use the following thermodynamic data for Mn to answer the questions below:

    Mn has four solid phases, α, β, γ, and δ:

    $$\overline{C}_p^{\alpha} = 21.6 + 15.9 \times 10^{-3} T \frac{J}{K \cdot mole} \qquad T_{trans}^{\alpha \to \beta} = 993K \qquad \Delta\overline{H}_{trans}^{\alpha \to \beta} = 2{,}010 \frac{J}{mole}$$

    $$\overline{C}_p^{\beta} = 34.9 + 2.8 \times 10^{-3} T \frac{J}{K \cdot mole} \qquad T_{trans}^{\beta \to \gamma} = 1373K \qquad \Delta\overline{H}_{trans}^{\beta \to \gamma} = 2{,}300 \frac{J}{mole}$$

    $$\overline{C}_p^{\gamma} = 44.8 \frac{J}{K \cdot mole} \qquad T_{trans}^{\gamma \to \delta} = 1409K \qquad \Delta\overline{H}_{trans}^{\beta \to \gamma} = 1{,}800 \frac{J}{mole}$$

    $$\overline{C}_p^{\delta} = 47.3 \frac{J}{K \cdot mole}$$

    a. Calculate the final temperature of the sample.

    b. Calculate the total enthalpy change for this process.

    c. Calculate the total entropy change for this process.

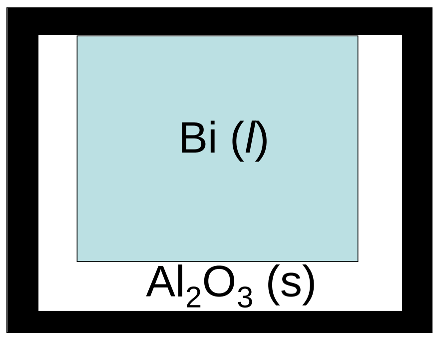
    d. What phase (or phases) are present at equilibrium at the end of this process?

11. Twenty kg of liquid bismuth at 600 K is introduced into a 10 kg alumina (Al_2O_3) crucible (initial temperature 298K), filling the crucible to the top; the crucible and bismuth are then surrounded by adiabatic walls (illustrated below). At equilibrium, according to the zeroth law, the temperatures of the bismuth and alumina crucible must be equal. Use the following thermodynamic data to answer the questions below:

$$\overline{C}_p^{alumina,solid} = 106.6 + 0.0178T \frac{J}{K \cdot mole} \qquad T_m^{alumina} = 2327K$$

$$\overline{C}_p^{Bi,solid} = 18.8 + 0.023T \frac{J}{K \cdot mole} \qquad T_m^{Bi} = 544K$$

$$\overline{C}_p^{Bi,liquid} = 20 + 0.00615T \frac{J}{K \cdot mole} \qquad \Delta\overline{H}_m^{Bi} = 10,900 \frac{J}{mole}$$



a. What is the final temperature of the system?

b. How much heat is transferred to the alumina?

c. At the final equilibrium, is the bismuth liquid or solid?

d. Consider now the same process, except that the adiabatic walls are removed. The closed system (can exchange heat…) of the bismuth in the alumina container is placed in a large room at T = 298 K, which behaves as a heat reservoir- it can transfer heat out of the system (or into it, depending on the temperatures of the reservoir and the system). At equilibrium, the bismuth and alumina will reach a final temperature of 298 K to match the environment of the room. How much heat will leave the bismuth to reach equilibrium?

12. Magnetic resonance imaging (MRI) is a common medical technique used for diagnostic imaging of tissues in patients. MRI is based on measuring the response of the weak magnetic dipoles in the atoms of tissues under a strong applied magnetic field. Typically, the magnetic induction in a clinical MRI machine may be ~2 Tesla. Consider the materials used to fabricate the MRI chamber that will be placed in the magnetic field, such as aluminum.

    a. What magnetic field strength is required to achieve a 2T induction in the MRI housing if the housing is fabricated from aluminum?

b. Will the magnetization induced in the aluminum be significant compared to, say, an iron permanent magnet that has a maximal net magnetization of 1.39×10^5 A/m? Support your answer with a calculation.

c. What is the work performed by the magnetic field in the volume of a section of the MRI aluminum housing 1 m x 1 m and 5 mm thick?