Problem set 1, due on September 22, **before** the beginning of the lecture

1 Energy scales in spectroscopy; units and their conversion (7 points, 1 for each subproblem)

Spectroscopical methods deal with the study of the interaction between electromagnetic (EM) radiation or a particle field (e.g. consisting of neutrons or electrons) and matter, with the goal to study its structural, electronic or other properties.

The amounts of energy (quanta) necessary to excite individual atoms or molecules, or "collective" motion like vibrations (phonons) in condensed matter is very small compared to everyday energy amounts, where the latter are measured in Joule (J). Therefore, energy units specific to the microscopic world, or the wavelength or frequency of the corresponding EM radiation, are often used.

a) One electron volt (1 eV) is defined as the kinetic energy an electron acquires when accelerated through an electrostatic potential of one volt. How much is 1 eV in J?

b) The energy of one energy quantum of radiation with frequency ν is $E = h\nu$, where h is the Planck constant. What is the frequency of EM radiation corresponding to 1 eV? What is the wave length λ of this radiation? Is this radiation visible to the human eye? If yes, which color does it correspond do? If no, how is the spectral range called to which this radiation belongs?

c) Often, the reduced Planck constant $\hbar = h/2\pi$ is used, resulting in $E = \hbar\omega$, where $\omega = 2\pi\nu$ is the angular frequency. The (angular) wave vector $\mathbf{k}$ is defined as a vector pointing in the propagation direction of a plane wave, having the magnitude $k = 2\pi/\lambda$; k is called the wave number. What is the relation between E and k? (iv) In spectroscopy (light scattering), scientists unfortunately often use a slightly different definition for the wave number omitting the factor 2π: $\tilde{k} = 1/\lambda$. Which $\tilde{k}$ corresponds to 1 eV? Provide your results in units of cm^{-1}.

(Side remark: A wave vector can be defined in an analogous way for any quantum object represented by a wave function, like the neutrons we will later introduce in neutron scattering to study the structure and vibrations of crystals. While the relation between E and k is linear for light, $E \propto k^2$ in massive particles.)

To have a reference, we will now review some typical energies from nuclear physics.

d) Calculate the rest energy of a proton having the mass $\sim 1.673 \times 10^{-27}$ kg, in J and eV. Hint: Einstein...

e) In the fusion of a Deuterium and Tritium, a neutron with a kinetic energy of 14.1 MeV (1 MeV, one mega electron volt $=10^6$ eV) is released. Calculate the velocity of the neutron.

f) In the spontaneous decay of $^{60}_{27}\mathrm{Co}$ to $^{60}_{28}\mathrm{Ni}$, two gamma quanta of energies 1.17 and 1.33 MeV are released. What is their wavelength and frequency?

Now we will discuss the typical energy scales observed in atoms and molecules.

g) In class we learned that a typical laboratory X-ray tube produces X-ray radiation by hitting a metal target with electrons, which can remove electrons from the inner shells. The vacancy is filled by electrons from shells lying further outside, emitting typical radiation; a typical wavelength observed when using copper targets is ~ 0.154 nm, so called K-α radiation. What frequency and energy in eV does this correspond to?

2 A little bit of chemistry and bonding types (7 points)

Six elements coded A, B, C, D, E and F, having atomic numbers (not necessarily in the order given) 1, 8, 10, 13, 19 and 35, form a series of stable compounds E_2B, D_2B, B_2, F_2B_3, FC_3, C_2, DC, EC and E_2 (A refuses to form a compound).

Using the periodic table, identify the elements and give the involved bonding types at ambient conditions. If the compound consists of molecules, give in addition the kind of force which acts between the molecules in the liquid/solid phase. (Possible answers could be, for instance: (i) The compound forms a crystal with ionic bonds; or (ii) The compound forms covalently bonded molecules which interact via van-der-Waals forces.) What bonding exists in the condensed form of A?

3 Internal energy of a liquid (8 points, group exercise)

Remark: This exercise is to be solved in groups of 3-4 students. Only one copy per group is to be submitted, with the names of the group members on it. While the idea is that you should help each other to solve it, at the end, when submitting the solution, everybody in the group should have understood and be able to explain the solution.

In the prereading / class we discussed the pair distribution function $g(\mathbf{r})$. Assume $g(\mathbf{r}) = g(r)$.

a) Which of the symmetry properties discussed in class does this imply?

b) If the liquid consists of atoms or spherical molecules such as CCl_4, the interaction potential between two such particles $u(r)$ will have the same symmetry. What is an example for such a potential?

c) Before proceeding to calculate the internal energy of such a liquid, let's have a look at the simple case of the ideal gas. How is this gas defined in thermodynamics? Do the particles in the ideal gas exert forces onto each other, i.e. do they interact? What is the internal energy of the ideal gas, $E = E_{kin} + E_{pot}$ and what are the individual terms E_{kin} and E_{pot}?

d) Now, let us turn to calculating the internal energy of the liquid, for which the interaction potential is given by $u(r)$. To which term of the internal energy $E = E_{kin} + E_{pot}$ does the interaction between the particles contribute? What is $E = E_{kin} + E_{pot}$ in terms of $g(r)$, $u(r)$ and the temperature T? You do *not* need to replace $g(r)$ and $u(r)$ by actual functions, e.g. the one you suggested in b).