Phys 155, Winter 2007, Homework 1, due Jan 17

(Each problem is 4 points. For problems from the textbook, please note that solutions are included in the textbook. However, use those solutions simply as guide, if necessary. If you do, your answers should show enough details that reflect your own understanding.)

1. Problem 1.6 of H&H

2. Problem 1.7 of H&H

3. In order to satisfy the Bragg condition, the wavelength λ of a probing particle need to be on the order of, or smaller than, the lattice spacing d. Since the typical lattice spacing of a crystal is a few Å, the wavelength of about 1 Å can be taken as a typical required value. Find corresponding energies in unit of eV (electron volt) when the probing particle is (a) a photon, (b) an electron, and (c) a neutron. (d) Which particle can be described as "thermal" in the sense that its energy is on the order of the room temperature 300 K (think the equipartition energy 3 $k_BT/2$). You may find useful the following fundamental constants: $\hbar c$ = 2.0E-5 eV cm, k_B = 8.6E-5 eV/K, m_ec^2 = 0.51E6 eV, m_nc^2 = 9.4E8 eV.

4. The classroom demonstration of a diffraction using laser was mimicking diffraction off of a two-dimensional crystal, important subject in surface physics/chemistry labs. It's interesting to consider this problem in detail. For instance, let's consider a hexagonal lattice (e.g. graphene lattice). Let the nearest neighbor distance of the lattice be *a*, and the wavelength of laser be 7000 Å (red light). We will use the unit cell convention as in the textbook (Figure 1.1(b)). Let's consider a diffraction spot coming from lines (21). (This is Miller index, and note that line in 2d corresponds to plane in 3d) (a) Using the lattice points shown exactly as in Figure 1.1(b), draw all identifiable (21) lattice lines. (b) What is the inter-line distance, d? (c) Consider an experimental situation, identical to that in class, that light impinges normal to the hexagonal lattice plane, and emerges on the other side *with an angle change*, which we may call Θ, due to diffraction off of (21) lattice lines. Derive Bragg's law for this situation. It will help to draw a diagram, representing each (21) line as a small circle, using the geometry where the lines are perpendicular to your paper. (d) What is the required distance *a* for the first order (i.e. n = 1 in Bragg's law) diffraction spot from (21) lines to appear at 0.25 in from the center when the distance from the lattice to the screen is 8 in? [Optional: After doing this problem, do you feel that there is some explanation missing about Figure 1.16a of H&H?]

5. Even closed-shell atoms such as Ne or Ar interact with each other via the van-der-Waals interaction, which is the interaction of two fluctuating electric dipoles ($1/R^6$), as opposed to the interaction of two static electric dipoles ($1/R^3$). This attraction, balanced by the hard-core repulsion, is the origin of the cohesive energy of van-der-Waals crystals. In this problem, let's try to understand how the $1/R^6$ attraction comes about. For simplicity, let's consider two

hydrogen atoms, hydrogen atom 1 and hydrogen atom 2, placed at vector **R** from hydrogen 1, where |**R**| is much larger than the Bohr radius.

(1) Suppose we take a snapshot measurement of positions of electrons 1 and 2, bound to atoms 1 and 2 respectively. We assume that protons 1 and 2 are at fixed positions, origin and **R** respectively. *Without* using any equations, explain why the lowest-order instantaneous Coulomb interaction between hydrogen 1 and hydrogen 2 is a dipole-dipole interaction.

(2) Using known results of E&M, write down the form of this interaction energy in terms of **R**, $\mathbf{r}_1$ and $\mathbf{r}_2$, where $\mathbf{r}_1$ is the position of electron 1, and $\mathbf{r}_2$ is the position of electron 2, both measured relative to the position of their respective partner protons. Do not derive any formula. Simply use your favorite E&M book (or use Google) to find the electric field **E** due to a dipole, and use the fact that the energy of another dipole $\boldsymbol{\mu}$ in that field **E** is $-\boldsymbol{\mu}\cdot\mathbf{E}$. How does this energy depend on R?

(3) The energy expression obtained in (2) gives the perturbation Hamiltonian operator H' of two weakly interacting hydrogen atoms. The unperturbed ground state wave function can be simply written as $|0\rangle = |1s\rangle_1|1s\rangle_2$, where the subscript 1 means hydrogen 1 etc. (In principle, the wave function should be written in ways to take into account of the identical nature of electrons 1 and 2, and all conclusions here remain true even if we do that, but here we for simplicity assume electrons 1 and 2 as non-identical.) Simply from the spherical symmetry of the 1s orbital, show that the first order perturbation correction to the energy eigenvalue vanishes.

(4) Show that the 2^{nd} order perturbation correction is finite, is negative and goes as $1/R^6$. In doing so, write down the wave function, or wave functions, of the first excited states that contribute to the 2^{nd} order correction, in the bracket notation given above. Again, do this without doing any actual integral calculation for matrix elements of H', but only by noting symmetry of involved orbitals and H'.

[Note: Although done for hydrogen atoms for simplicity, this proof of the form of van-der-Waals interaction is readily generalized for any neutral non-diploar objects interacting at a large distance.]

[Hint: This is what is meant by the "symmetry property." As you learned from quantum mechanics or modern physics or introductory chemistry, an s orbital wave function depends on the radial distant r only, while wave functions for p orbitals, i.e. px, py, pz orbitals, depend on (r, x), (r, y), and (r, z), respectively. Thus, s orbitals remain unchanged by all reflection operations (e.g. reflection which is substitution by x -> -x), rotations or inversion. However, p orbitals do change under some of these operations. Consideration of changes of p orbitals under reflections (e.g. x->-x in the integral) or inversion would be sufficient to examine whether matrix elements in the perturbation expression vanishes or not.]