

ECE 4070: Physics of Semiconductor and Nanostructures

Spring 2014

Exam 1

March 13, 2014

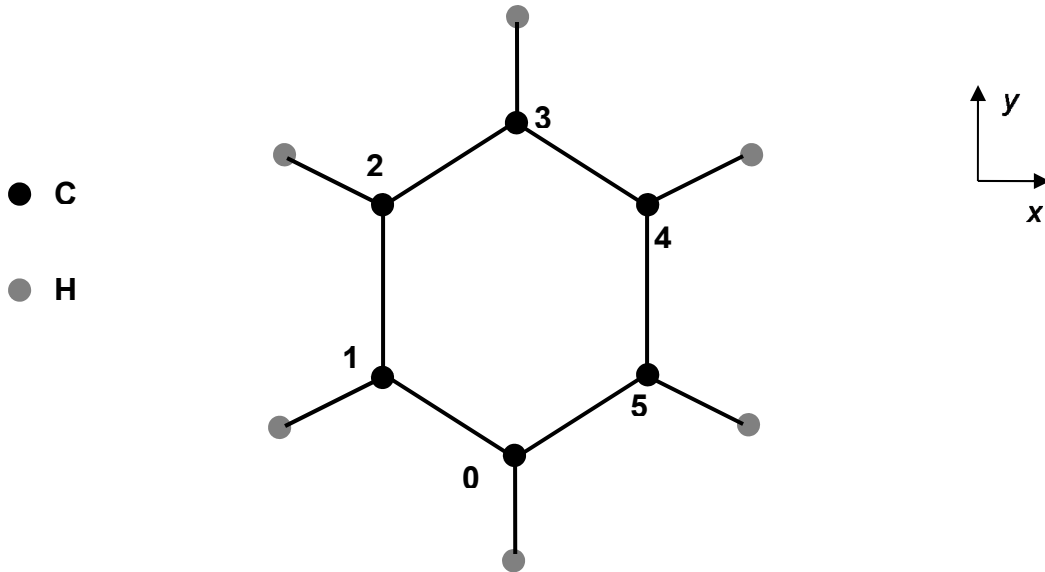
INSTRUCTIONS:

- Every problem must be done in the blue booklet
- Only work done on the blue exam booklets will be graded – do not attach your own sheets to the exam booklets under any circumstances
- To get partial credit you must show all the relevant work
- Correct answers with wrong reasoning will not get points
- All questions do not carry equal points
- All questions do not have the same level of difficulty

DO NOT WRITE IN THIS SPACE

Problem 1 (Benzene molecule) – 40 points

Consider the Benzene molecule C_6H_6 shown below:



In Benzene molecule each carbon atom is sp^2 hybridized and forms sp^2 - sp^2 sigma bonds with two neighboring carbon atoms and one sp^2 - s bond with a hydrogen atom. This leaves one p_z orbital on each carbon atom. This p_z orbital sticks out of the plane of the molecule and forms pi-bonds with the p_z orbitals on neighboring carbon atoms. The goal of this problem is to find the wavefunctions and the energy levels that result from the p_z orbitals. Let the position vector of the n -th carbon atom be \vec{r}_n and let the p_z orbital sitting on the n -th carbon atom be $|\phi_{pz}(\vec{r} - \vec{r}_n)\rangle$. Let the energy of the p_z orbital be E_p and the energy matrix element between neighboring p_z orbitals be $-V_{pp\pi}$.

a) How many molecular orbitals (and corresponding molecular energy levels) would result from the p_z orbitals? **(10 points)**

Suppose one tries a variational LCAO wavefunction of the form: $|\psi(\vec{r})\rangle = \sum_{n=0}^5 c_n |\phi_{pz}(\vec{r} - \vec{r}_n)\rangle$:

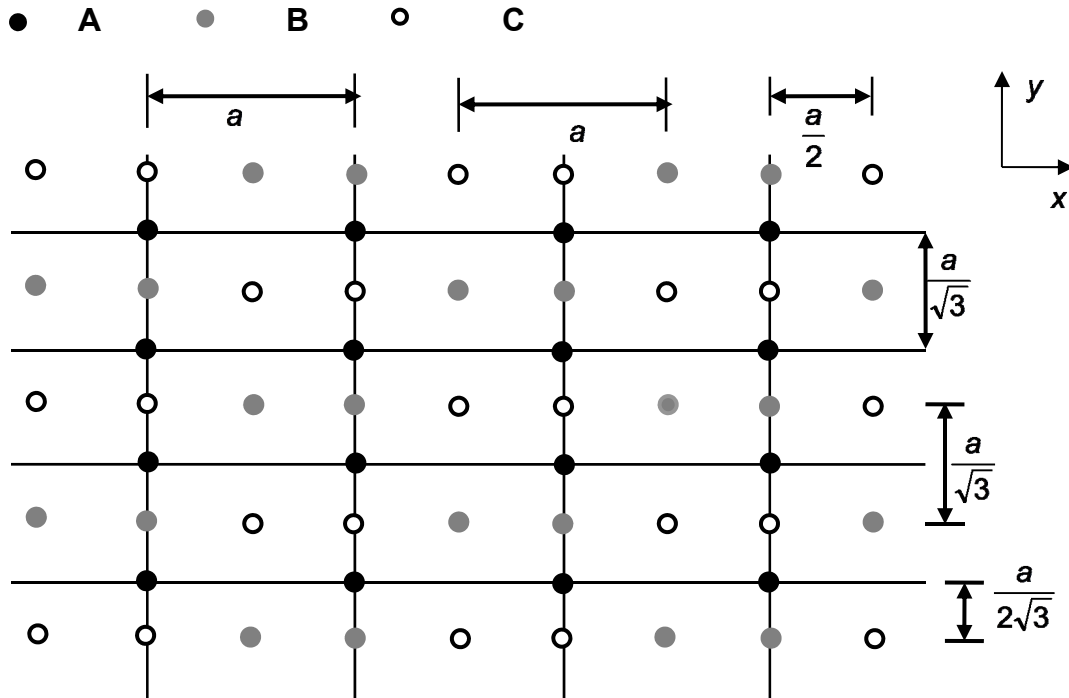
b) Obtain a matrix equation whose solution would give the desired energy levels and the corresponding values of the coefficients c_n . **(10 points)**

c) Show that, $c_n = \frac{e^{i n s}}{\sqrt{6}}$, where s is a constant, satisfies the matrix equation obtained in part (c) provided s is allowed to have only certain values. What are the values that s can have? **(10 points)**

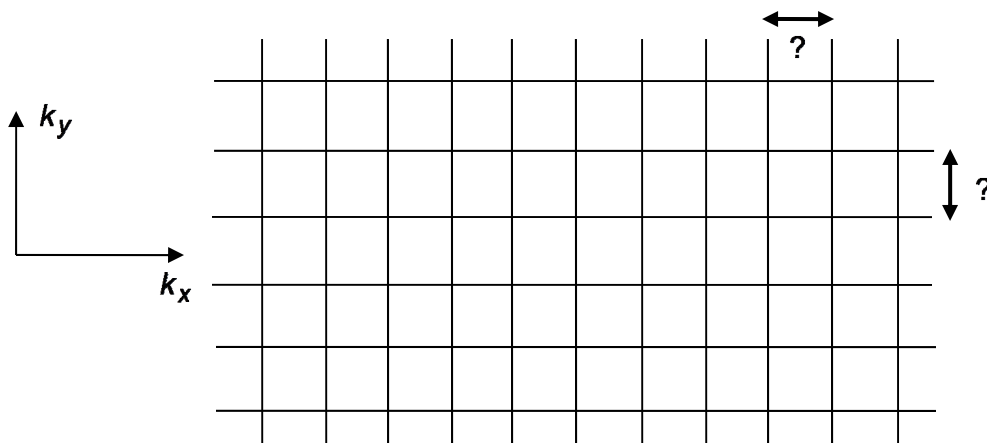
d) Find the energies of all the molecular orbitals that result from the p_z orbitals. **(10 points)**

Problem 2 (2D lattice) – 30 points

Consider the following lattice consisting of three different kinds of atoms: A-atom (black-filled), B-atom (gray-filled), and C-atom (black-unfilled).



- Find and give expression for the primitive lattice vectors \vec{a}_1 and \vec{a}_2 and draw them on the figure and submit the figure with your exam copy. **(10 points)**
- Sketch the Wigner-Seitz primitive cell for the lattice on the figure and submit the figure with your exam copy. **(5 points)**
- How many A-toms, how many B-toms, and how many C-atoms are in one Wigner-Seitz primitive cell? **(5 points)**
- Sketch the reciprocal lattice on the **rectangular** grid provided below in the figure by black dots and label the vertical and horizontal dimensions of the grid where question marks are shown. Submit this figure with your exam copy. **(10 points)**



Problem 3 (Electron gas in two dimensions) – 30 points

Parts (a), (b) and (c) are unrelated.

a) Consider a **free electron gas in 2 dimensions at near-zero temperature**. The number densities of spin-up and spin-down electrons are equal and both equal half the total electron density (i.e. $n_{\uparrow} = n_{\downarrow} = n/2$).

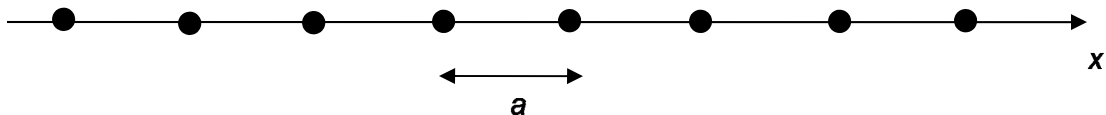
Now suppose a magnetic field is turned on and it points in the +z direction (i.e. $\vec{B} = B_0 \hat{z}$). Here we will only concern ourselves with the interaction between the electron spin and the magnetic field. In the presence of the magnetic field the Hamiltonian is given by,

$$\hat{H} = \frac{\hat{P} \cdot \hat{P}}{2m} + 2\mu_B \hat{\sigma}_z B_0$$

where μ_B is a constant called the Bohr magneton, and $\hat{\sigma}_z$ is the spin operator with eigenvalues equal to +1/2 and -1/2 for spin-up and spin-down electrons, respectively. So spin-up electrons with wavevector \vec{k} have energies $E_{\uparrow}(\vec{k})$ given by $\hbar^2 k^2 / 2m + \mu_B B_0$ and spin-down electrons with wavevector \vec{k} have energies $E_{\downarrow}(\vec{k})$ given by $\hbar^2 k^2 / 2m - \mu_B B_0$. Now find the difference between the number density of spin-down and spin-up electrons. There should be no unevaluated integrals in your answer. **(10 points)**

Hint: The chemical potential or the Fermi level for both spin-up and spin-down electrons must be the same in thermodynamic equilibrium.

b) Consider a one-dimensional crystal shown below.



At each lattice site there is one atom that has a single s-orbital that contributes to bonding. The resulting energy band dispersion is:

$$E(\vec{k}) = E_s - 2V_{ss\sigma} \cos(k_x a)$$

Find the 1D density of states $g_{1D}(E)$ that will let you convert an integral over k -space for this energy band to an integral over energy-space and **plot** $g_{1D}(E)$ as a function of the energy E .

(10 points)

c) In a certain 2D crystal the energy band dispersion of the electrons is given by the formula:

$$E(\vec{k}) = \hbar v \sqrt{k_x^2 + k_y^2}$$

Find the 2D density of states $g_{2D}(E)$ that will let you convert an integral over k -space for this energy band to an integral over energy-space and **plot** $g_{2D}(E)$ as a function of the energy E .

(10 points)