Physics 555 **Fall 2007** **HW 1**

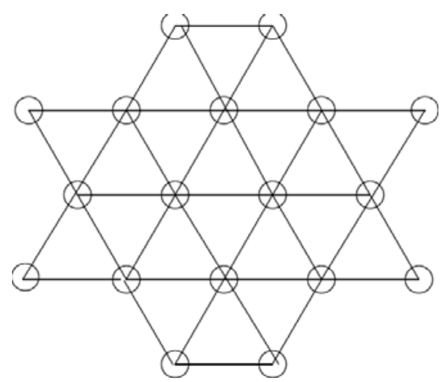
due Wednesday Sept 10

Read Ziman, Ch. 1. I suggest some slight changes in the text.

(1) Page 12 item (v) should indicate that the shape of the Brillouin zone can be chosen in various ways, of which the simplest is a paralleliped defined by the triad $(\vec{b}_1, \vec{b}_2, \vec{b}_3)$. The more symmetrical Wigner-Seitz choice is the usual conventional choice, but is not unique. I may use a slightly different notation from Ziman, where $(\vec{a}_1, \vec{a}_2, \vec{a}_3)$ is replaced by $(\vec{a}, \vec{b}, \vec{c})$, and $(\vec{b}_1, \vec{b}_2, \vec{b}_3)$ is replaced by $(\vec{G}_1, \vec{G}_2, \vec{G}_3)$ or $(\vec{A}, \vec{B}, \vec{C})$. When the term "Brillouin zone" is used, one can assume that this means what Ziman calls the "first Brillouin zone" or the "reduced Brillouin zone," unless it is explicitly stated otherwise.

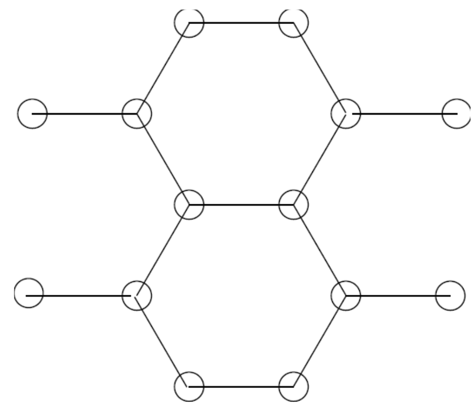
(2) Page 17, the statement of Bloch's theorem in italics should read "*When choosing a complete set of eigenfunctions of a translationally-invariant linear equation like the Schoedinger equation, it is possible to choose them all to be simultaneous eigenfunctions of the translations, such that translation by a lattice vector* $\vec{\ell}$ *is equivalent to multiplying by a phase factor of the type* $\exp(i\vec{k}\cdot\vec{\ell})$, *where* $\vec{k}$ *is a vector lying in the Brillouin zone and consistent with the boundary conditions.* Ziman says it very concisely on the bottom of p. 19.

1. A primitive 2d lattice consists of a sheet of close-packed atoms forming a triangular lattice. A fragment is shown to the right. The actual sample extends to infinity ("horizontally") and is a single layer thick "vertically." **(a)** What are the primitive translation vectors (pick two permissible sets, one with sensible short vectors and the other not.) **(b)** What are the corresponding reciprocal lattice vectors? Draw the reciprocal lattice in a diagram similar to the one on the right, with spatial x and y coordinates corresponding correctly. Note that either choice of reciprocal lattice basis vectors (the one following from the sensible primitive translations, and the other one) generate the same reciprocal lattice. **(c)** This sheet of atoms lives in a 3d world in which it can translate and rotate, etc. In addition to translational symmetry, this lattice has also some "point symmetry." These are symmetry operations that leave at least one point fixed in space. Counting the identity operation, there are 12 "proper" rotations. What are they? Note that the symmetry operations have a natural multiplication, and form a group. Write out the multiplication table for rotations around a vertical axis. **(d)** Show that not all proper rotations belonging to the "point group" of this object commute with each other. (e) Finally, there are 12 "improper" rotations. One of them, the inversion,



can also be expressed as a rotation by π around the vertical axis times a mirror reflection in the plane of the lattice. List the 12 improper rotations, in a simple format of mirrors possibly multiplied by rotations.

2. Graphite has hexagonal packing of atoms in planes, and a slightly complicated rule for stacking planes on top of each other. The vertical spacing is large and the bonding between planes is weak. In recent years it has been shown that single sheets of graphite (called "graphene") can be separated and mounted on fairly inert substrates where they can be studied. A fragment is shown at the right. **(a)** Choose a simple, symmetrical choice of primitive translations $\vec{a},\vec{b}$. **(b)** Find the corresponding primitive reciprocal lattice vectors $\vec{A},\vec{B}$. How many atoms are in a primitive unit cell? Note that not all point symmetries of the previous triangular lattice are available here. For example, no inversion leaving graphene unchanged can leave any atom fixed in space, but inversion through the hexagon center is a symmetry operation. Alternately, you can have an inversion center on an atom, and then "multiply by" a sub-primitive translation. **(c)** Explain this sub-primitive translation. The complete symmetry group contains as many non-pure translations as does the triangular lattice, but there is no simple separation into point operations times translation operations, where both the point operation and the translation operation are also symmetry operations by themselves. Such a space group is called "non-symmorphic."



3. For the hexagonal closed packed (hcp) structure, **(a)** what is the lattice and the basis? **(b)** If atoms are regarded as hard spheres, what should be the choice of axial ratio *c/a* to make the hard spheres touch? **(c)** what is the "packing fraction" (ratio of volume inside spheres to total volume). **(d)** what is the packing fraction of the fcc and the bcc crystal structures?