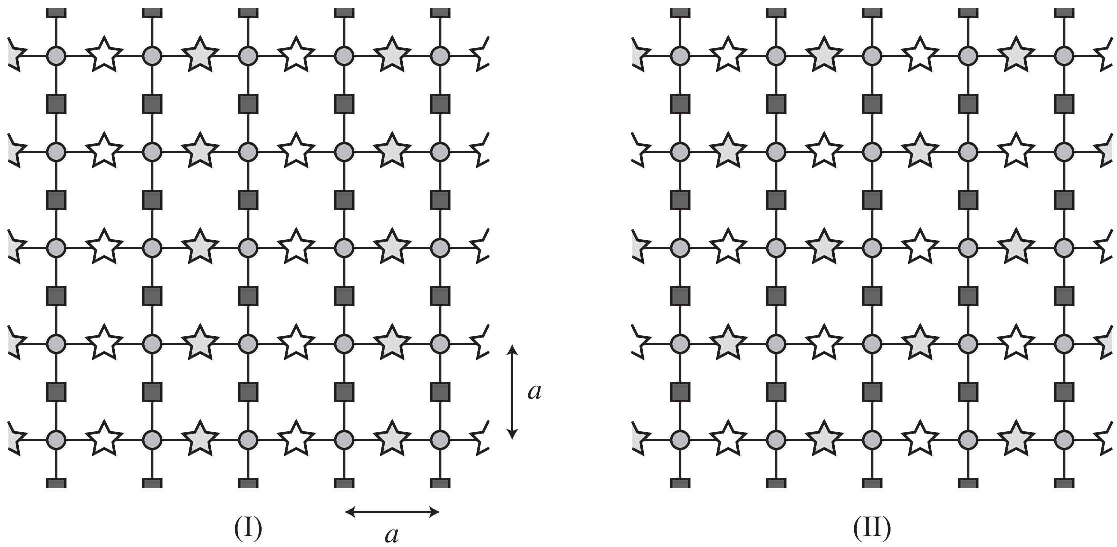
Physics 725: Assignment 1

(to be submitted by Thursday, January 31, 2019)

1. Consider the two-dimensional crystals labelled I and II.



Answer each of the following questions for <u>both</u> the type-I and type-II cases.

(a) Provide a set of lattice vectors $\{\boldsymbol{a}_1, \boldsymbol{a}_2\}$ that describes the Bravais lattice. *Hint:* Start from a particular atom and find the two shortest, non-collinear vectors that connect the atom to two equivalent ones in adjacent unit cells; equivalent here means the same atom in the same local environment.

(b) Introduce a dummy lattice vector $\boldsymbol{a}_3 = \boldsymbol{e}_z$, directed out of the plane of the crystal, and compute the area of the unit cell $\Omega_0 = (\boldsymbol{a}_1 \times \boldsymbol{a}_2) \cdot \boldsymbol{a}_3$.

(c) Construct a basis $\{\boldsymbol{\tau}\}$ for the atoms in each unit cell.

(d) Determine the corresponding reciprocal lattice vectors and identify the Brillouin zone (BZ) using the Wigner-Seitz construction.

(e) Indicate which of the following is a symmetry of the crystal:

- translation by $a\boldsymbol{e}_x$
- translation by $a\boldsymbol{e}_y$
- inversion through a point coinciding with a filled square
- rotation by $\pi/2$ through a point coinciding with a filled circle
- rotation by π through a point coinciding with a filled circle
- mirror reflection across a line running vertically through stars only
- mirror reflection across a line running diagonally through circles only
- translation by $a\boldsymbol{e}_x$ followed by a mirror reflection across a line running horizontally through squares only (an example of a *glide*)

2. Imagine a molecular rope made up of an alternating sequence of atoms A and B, where the AB bonding length is a constant value a.

   (a) Sketch this system and explain why it should be viewed as a crystal.

   (b) The atomic positions are given by $R_A = R + \tau_A = 2na$, and $R_B = R + \tau_B = (2n+1)a$, where n is an integer. Provide definitions of the lattice vectors and basis.

   (c) Give a definition for the reciprocal lattice $\{G\}$ and show that it is indeed reciprocal to the Bravais lattice $\{R\}$. The best way to do this is to prove that $\exp(iGR) = 1$ for all possible choices of G and R.

   (d) In the ground state, any physical properties of the system will share the periodicity of the lattice and admit an expansion

   $$f(r) = \sum_G f_G e^{iGr}.$$

   Show that $f(r+R) = f(r)$ for any R in the Bravais lattice.

   (e) What condition on the coefficients f_G ensures that $f(r)$ is real?

   (f) Consider a single electron living along the molecular rope. Argue that the most general form of its wave function is

   $$\psi(r) = \sum_G f_G e^{i[Gr+\theta(r)]}.$$

   (g) Show that

   $$\frac{1}{2a}\int_0^{2a} dr\, |\psi(r)|^2 = \sum_G |f_G|^2.$$