PHY460: Problem Set #2 Due: Friday 10/6 by 5pm in Yellow PHY460 homework box between Loomis and MRL on 2nd Floor

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1. Draw a 5x5 lattice of unit cells for a 2d lattice with Bravais lattice vectors:

   (a) $\vec{a}_1 = a\hat{x}$, $\vec{a}_2 = 2a\hat{y}$

   (b) $\vec{a}_1 = a\hat{x} + a\hat{y}$, $\vec{a}_2 = a\hat{x} - a\hat{y}$

   (c) For parts (a) and (b) identify whether the system has C_2 symmetry, C_4 symmetry or both. One out of the two has both. For the one with both mark on your drawing the two locations for C_4 rotation centers and the four locations for C_2 rotation centers. HINT: Two out of the four C_2 rotation centers coincide with the two C_4 rotation centers.

2. Consider the 2d lattice in Figure 1.

   (a) Re-draw the lattice for your solution. Then draw a box that encloses one unit cell.

   (b) How many atoms are in each unit cell?

   (c) There are three sets of lattice vectors (1,2,3) which one(s) can act as primitive vectors.

3. Consider a 1d lattice with 3 atoms per unit cell. Assume that two atoms are O(xygen) and the other **one** is Si(licon). Arrange the atoms in the unit cell such that the system has reflection symmetry. Draw 6 unit cells on a line and draw vertical lines through the allowed reflection centers.

4. Suppose that for a two atom system (crystal) that the potential energy is $U(r) = \epsilon\left[\left(\frac{\sigma}{r}\right)^5 - e^{-r/\xi}\right]$ where r is the relative distance between the atoms and ϵ, σ, ξ are constants.

   (a) What are the units of the constants ϵ, σ, and ξ?

   (b) Sketch the function $U(r)$ as a function of r assuming $\epsilon = \sigma = \xi = 1$. **Assume they take these values for the rest of the problem.**

   (c) Find the extrema of $U(r)$, and determine if they are minima or maxima through a second-derivative test. **HINT: The equation to determine the extrema (first derivative) is transcendental and must be determined either through plotting or numerically. I suggest using mathematica to get an approximate result. If you use mathematica or the graphical method show how you determined the extremal values *e.g.* show the plot of both sides of the transcendental equation.**

   (d) $U(r)$ has one minimum. Expand $U(r)$ around the minimum r_0 up to second order in $(r - r_0)$ *i.e.* keep terms of order $(r - r_0)^2$. Show that this form of the potential energy leads to a Hooke's law restoring force if the relative atomic distance is slightly disturbed from r_0 by an infinitesimal amount dr.

   (e) Now consider the case of 3-atoms. Assume the atoms sit a distance R away from each other at the points of an equilateral triangle. Determine the total potential energy of the system by summing up $U(r)$ for each pair. Minimize the total potential energy as a function of R to determine the equilibrium distance (lattice constant).

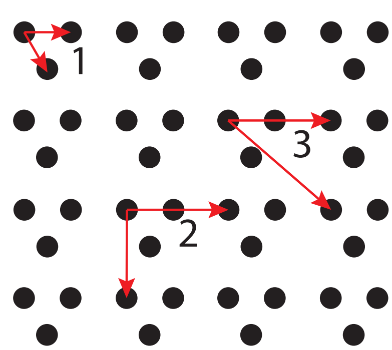

Figure 1: Lattice Structure for Problem 2