MSE 102, Fall 2012 Final Exam

Write your name here: _____

Instructions:

- Answer all questions to the best of your abilities. Be sure to write legibly and state your answers clearly.
- The point values for each question are indicated.
- You are not allowed to use notes, friends, phones, etc.
- You can use calculators.
- There are a total of 100 points.
- Feel free to ask questions, but only for clarification purposes.

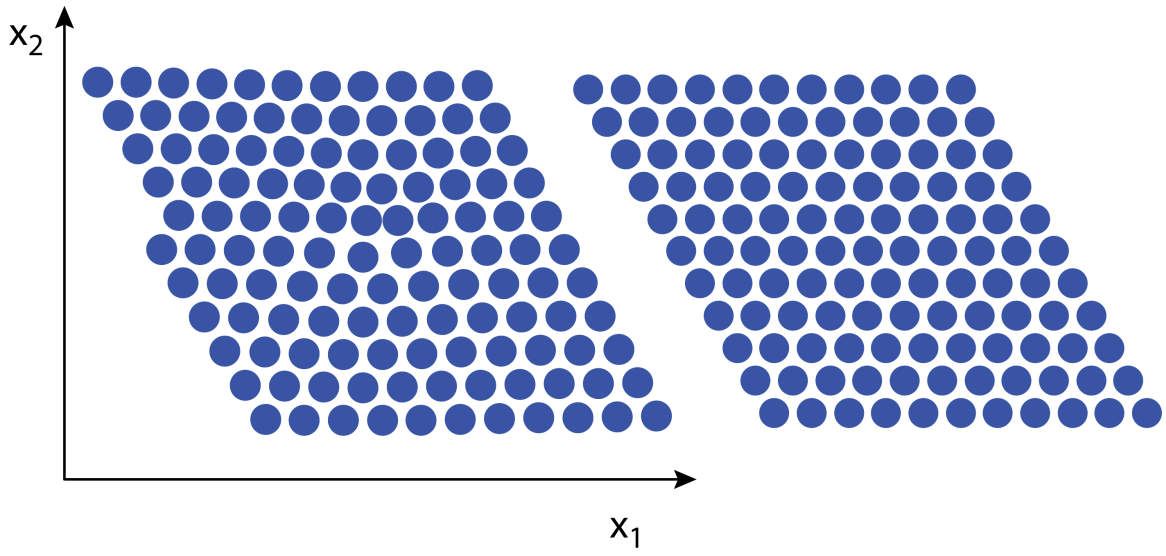
I hope you all do really well.

It was a pleasure teaching you.

- DCC

Problem Number	Score
1	/ 10
2	/ 10
3	/ 10
4	/ 10
5	/ 10
6	/ 10
7	/ 10
8	/ 10
9	/ 10
10	/ 10
Total	/ 100

1. The figure below (on the left) is part of a crystal containing a dislocation. The perfect crystal is displayed on the right. The x_3 direction points out of the page toward you, and conincides with six-fold axes of rotation in the perfect crystal.



(a) Remembering that a Burgers circuit is just path that circles the dislocation, construct the Burgers circuit for the dislocation on the left [2 points], and identify the Burgers vector on the right panel [3 points].

(b) (1 point) What is the line direction of the dislocation? [1 point] Give a vector that is normal to the slip plane of the dislocation.

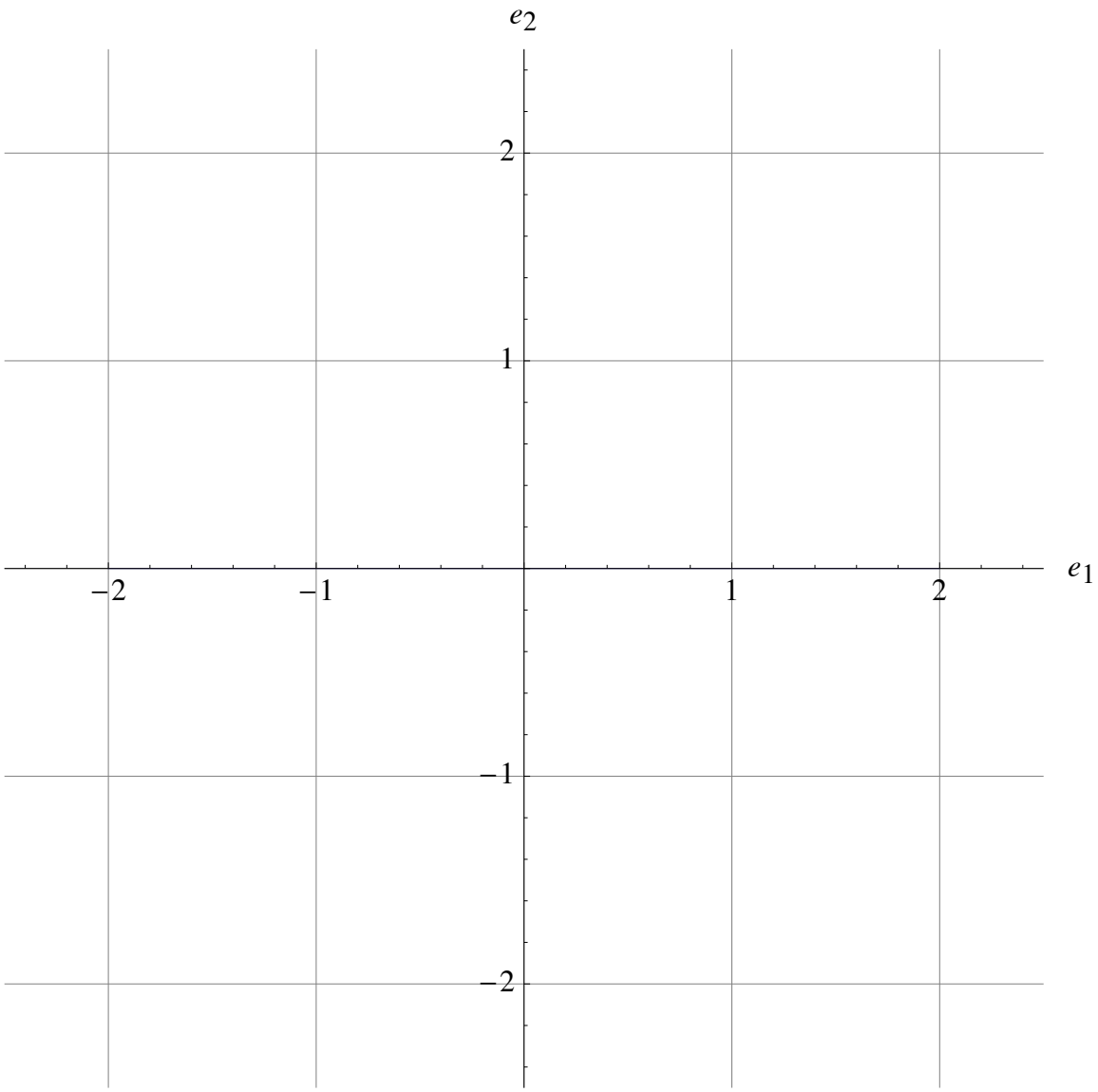
(c) Assume that the stress given below is applied to the crystal. [2 points] Compute the force exerted on the dislocation by the applied stress. [1 point] Assuming that the dislocation is only allowed to climb, in which direction does the dislocation move under the applied stress ? (Give an explicit vector describing the direction.)

Assume that $\sigma = \begin{bmatrix} \sigma_1 & \sigma_o & 0 \\ \sigma_o & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}$ with $\sigma_o > 0$ and $\sigma_1 > 0$ and that $|\mathbf{b}| = b$.

2. A 2D crystal has the symmetry *p2mg* (plane group 7). More specifically it is known that the crystal has C atoms at Wyckoff positions (d) and N atoms at positions (b). (In addition, it is known that there are other, unspecified, atoms within the unit cell.) The primitive lattice vectors are given by $\mathbf{a} = -2\pi\,\mathbf{e}_2$ and $\mathbf{b} = 2\pi\,\mathbf{e}_1$.

(a) [5 points] Construct the primitive reciprocal lattice vectors for this crystal, and sketch them on the axes on the next page. Define the reciprocal lattice vectors $\mathbf{G}_{hk}$, and plot their positions on the plot on the next page using an $\times$. Identify the reciprocal lattice point $2\bar{1}$.

(b) [5 points] Indicate the positions at which you expect to see diffraction from both the C atoms with a $\bigcirc$ and those with contributions from the C and the N atoms with a $\bigcirc$. (It is okay if these symbols obscure your $\times$'s denoting the reciprocal lattice points.)


e_2
2
1
−2
−1
1
2
e_1
−1
−2

3. An electron bound within a hydrogen atom is initially described by the wavefunction:

$$\Psi(\mathbf{r},t) = -\frac{3i}{5}\exp\left(\frac{-iE_4 t}{\hbar}\right)\psi_{420}(\mathbf{r}) - \frac{4}{5}\exp\left(\frac{-iE_1 t}{\hbar}\right)\psi_{100}(\mathbf{r}),$$

with $\psi_{nlm}(\mathbf{r})$ an eigenfunction of the Hamiltonian operator for the hydrogen atom.

(a) [2 points] Give the expectation value of the z-component of the angular momentum, $\hat{L}_z$, for the electron.

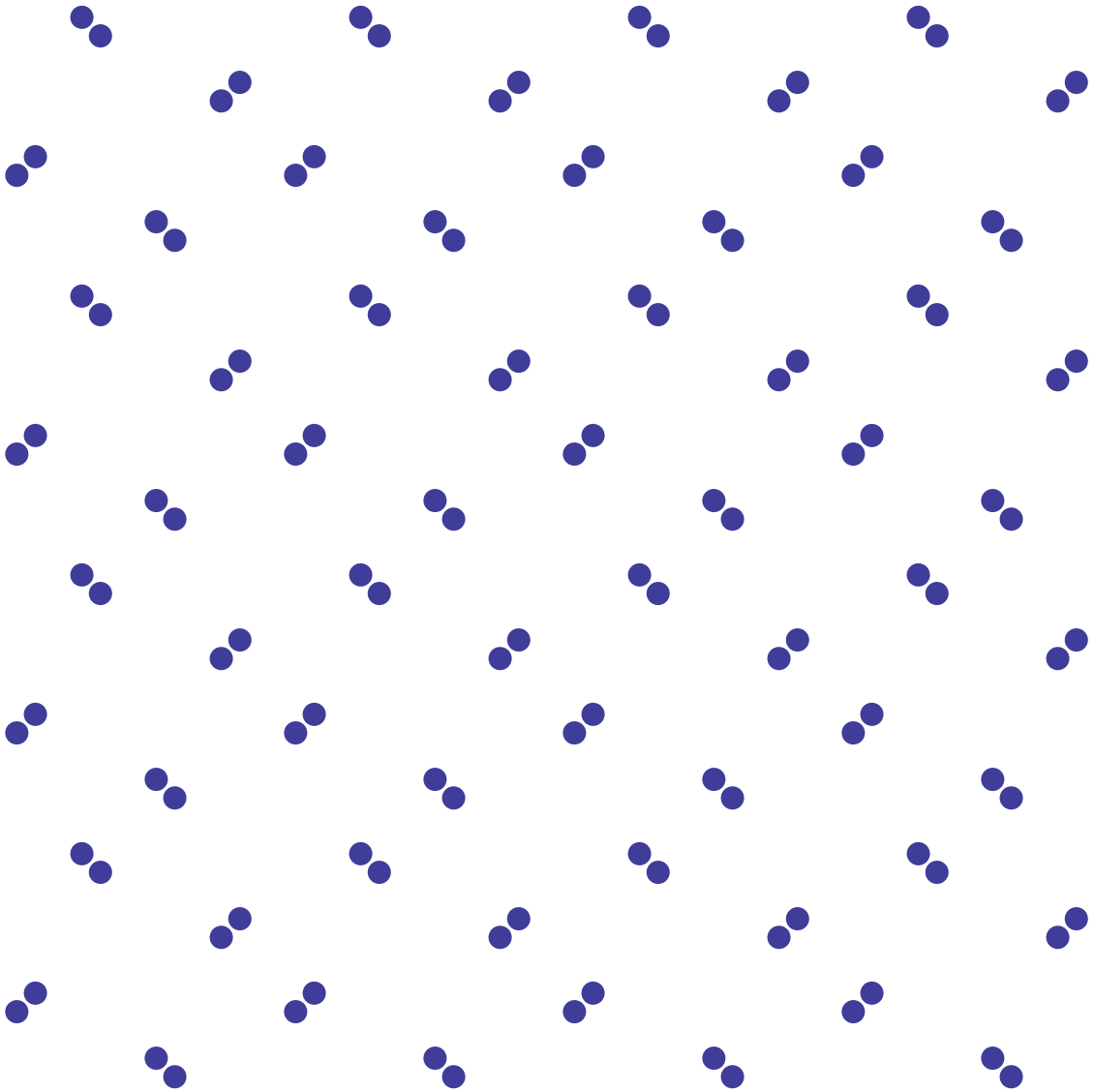
(b) [4 points] Give the expectation value of the total energy in eV. Recall that the Rydberg is 13.6 eV.

(c) [2 points] Give the expectation value of the angular momentum squared, L^2.

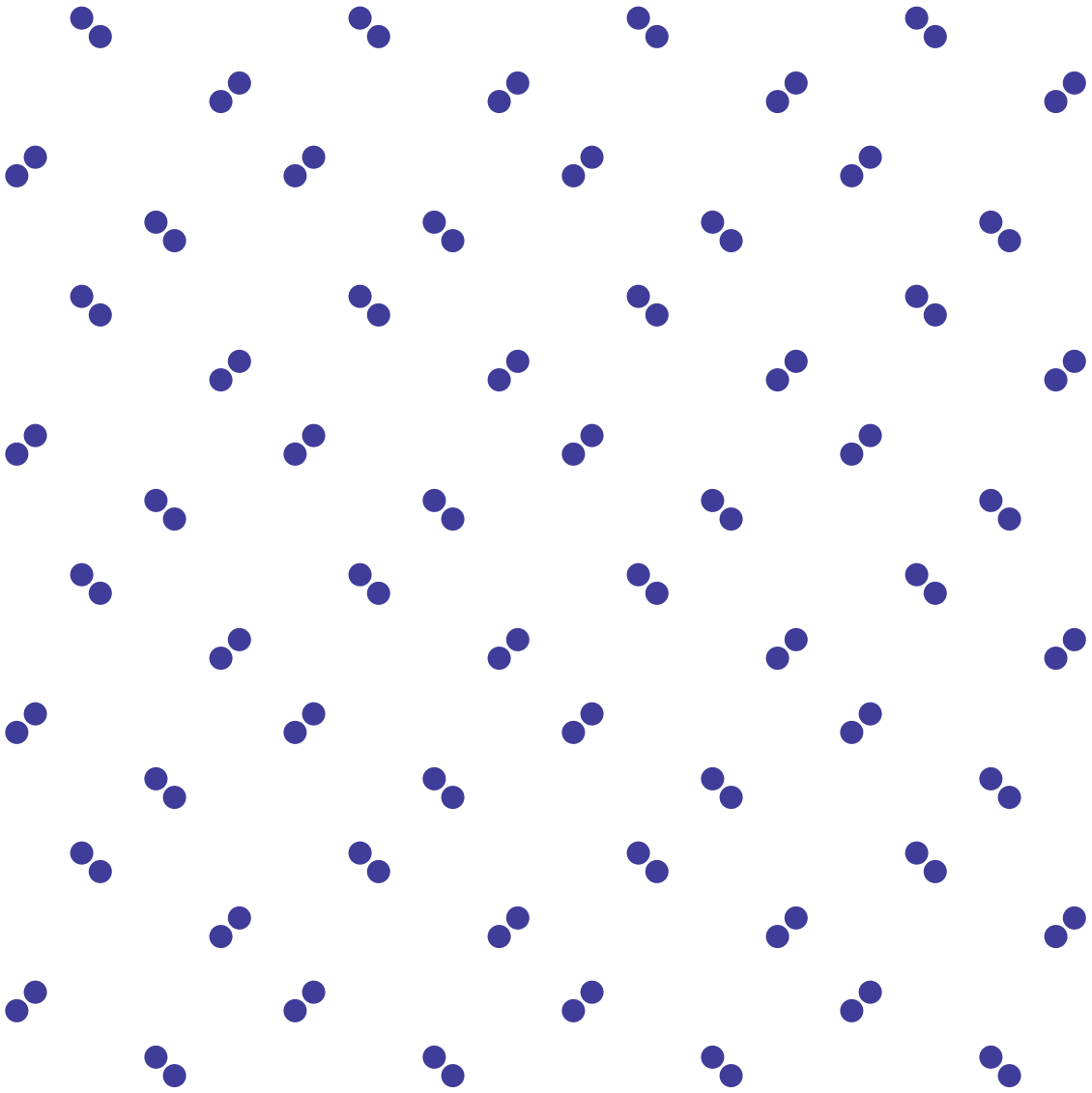
(d) [1 point] You set out to measure the position of the electron within the atom in the state as described above. Is the probability distribution describing this position time dependent? Why or why not?

(e) At time t_1, the energy of the H atom is measured to be E_4. [1 point] What will subsequent measurement of the energy at time $t_2 > t_1$ yield, presuming that no other properties of the electron are measured during the interval between t_2 and t_1?

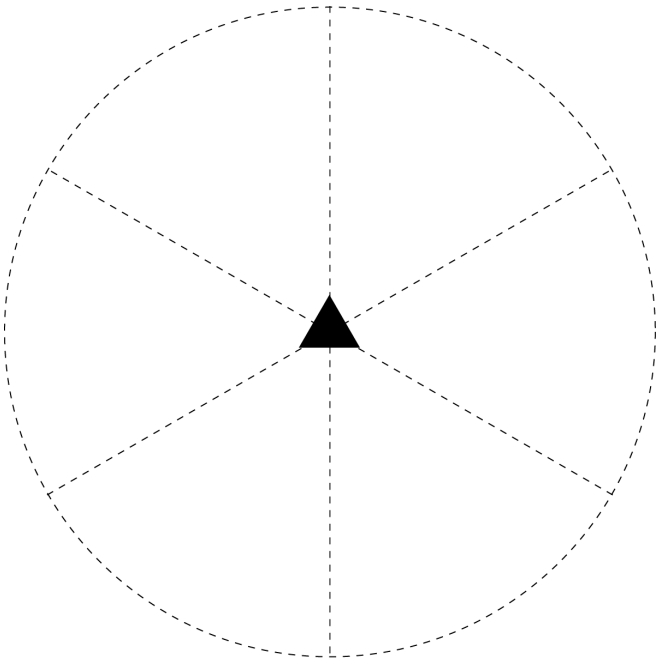
4. A 2D crystal has the structure shown in the figure. (I've included two copies of the figure so that you have room for all of the things you need to sketch.)



Use the plane group tables to help you:
[2 points] Identify a set of lattice points, marking each with an X.
[2 points] Identify a set of primitive lattice vectors.
[2 points] How many atoms are in each primitive unit cell?
[1 point] Label the point 12 defined by your choice of origin and primitive lattice vectors.
[1 point] Identify a unit cell.
[1 point] Indicate *all* of the symmetry elements within the cell.
[1 points] Give the plane group number/symbol, and sketch the asymmetric unit.

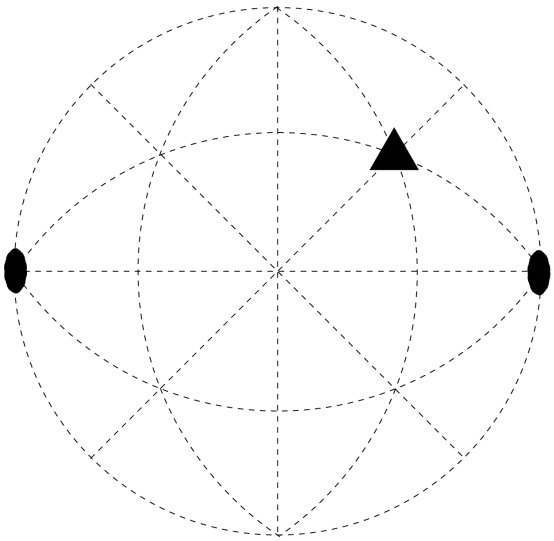


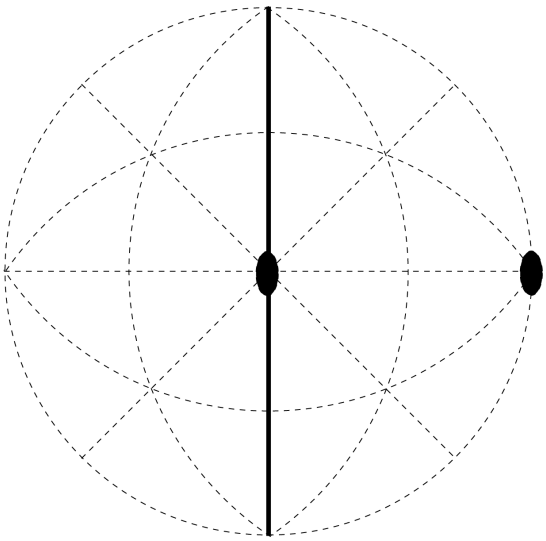
5. A crystal has the point symmetries (and all the associated implied symmetries) shown in the following stereogram.

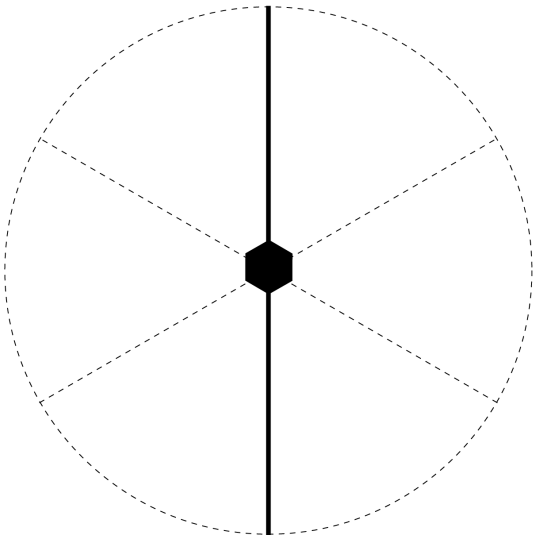


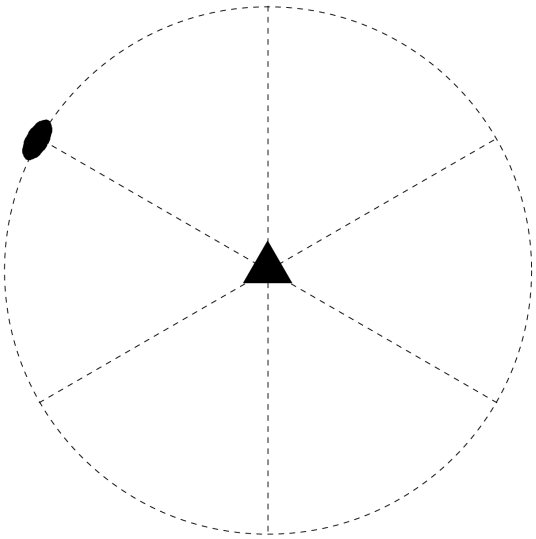
[10 points] Given this symmetry, what is the structure of a generic symmetric second rank tensor property for this crystal. Support your answer with a clear and mathematical argument.

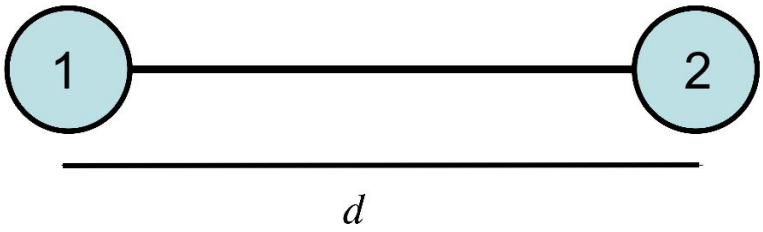
6. [2 points each = 8 total points] Complete the stereograms, including demarcating a set of points that are equivalent by symmetry. (None of the points in your set should lie on a symmetry element.) [2 points] List all of the symmetry elements defining the group displayed in the upper right stereogram. (That is, give a list of the individual elements forming the group.)











7. The Hamiltonian matrix for an electron bound to a dimer with bond length d, determined using a basis composed of the S states of the bare atoms, is given by:

$$\mathbf{H} = \begin{pmatrix} E_1 & -V_o \\ -V_o & E_2 \end{pmatrix}$$

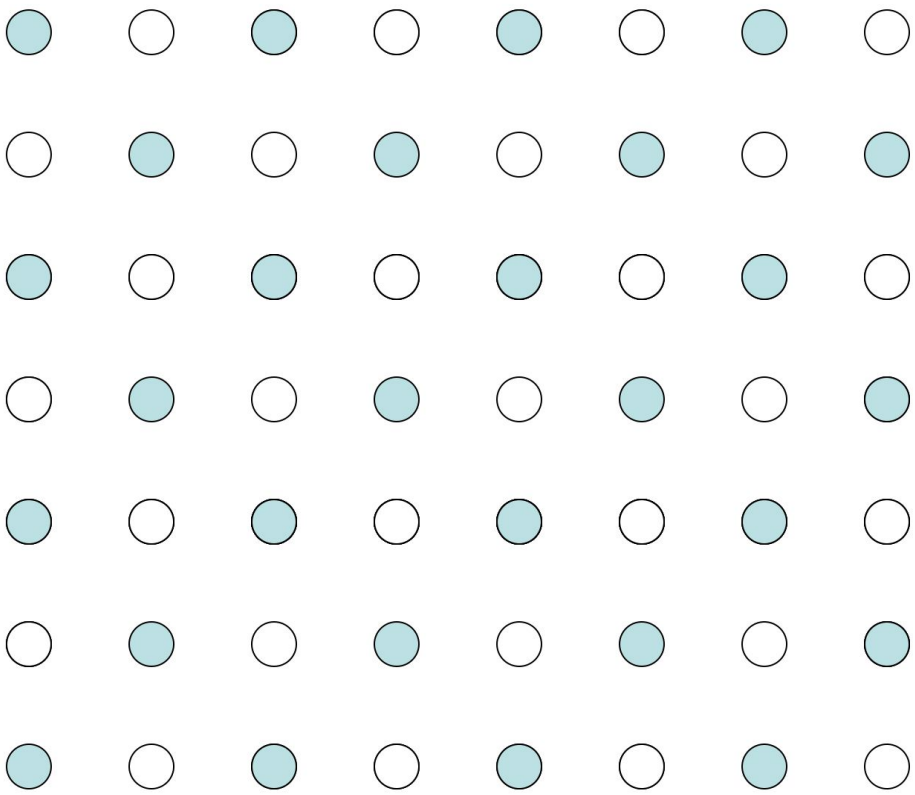
Here, E_1 and E_2 are the energy levels for an electron in the bare atoms labeled 1 and 2, respectively.

(a) [2 points] What energies may one measure for an electron bound to the dimer?

(b) [4 points] Sketch the eigenfunction associated with the *antibonding* state. Assume the atomic basis states are $\psi_{100}(\mathbf{r})$ states of the respective atoms. Assume that $E_2 = 8$ eV, and $E_1 = 3$ eV, and state in words how this is reflected in your sketch. (Plot the eigenfunction along the line connecting the nuclei of the dimer, as we did in class. There is no need to compute directly the eigenvectors – a sketch with the correct features will do.)

(c) Assume that $E_2 = 8$ eV, and $E_1 = 3$ eV and d is chosen such that $V_o = 2$ eV. [2 points] Sketch the energy level diagram for the dimer. [1 point] If there are two electrons in the molecule, one from each atom, what is the change in electronic energy associated with forming the bond? [1 point] Is the bond ionic, covalent or somewhere in between? Explain your answer making reference to the parameter $\delta \equiv \frac{E_2 - E_1}{2V_o}$.

8. A two-dimensional ionic crystal appears as shown in the sketch.



Assume that the darker atoms are Ca atoms (atomic number 20, in the same column of the periodic table as Mg), and the white atoms are S (atomic number 16, in the same column as O. Assume that the repulsive part of the atom interaction is given by the repulsive part of the Lennard-Jones potential with the parameters $\sigma = 4$ Å and $\varepsilon = 0.01$ eV, and that the attractive part stems solely from the modified Coulomb interactions between the ions given above.

[5 points] Compute the repulsive part of the Lennard-Jones potential for this crystal (per lattice site) assuming that the nearest neighbor distance between ions is $d_o = 1.25$ Å. You will need the following sum:

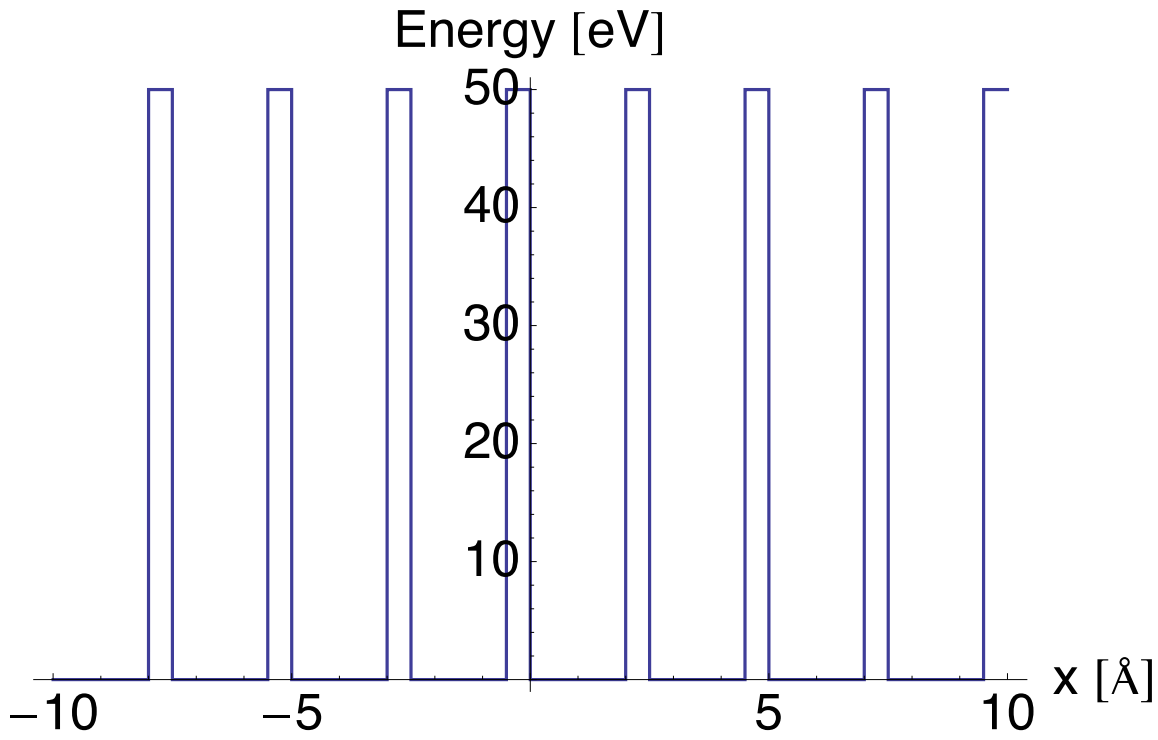
$$\sum_{u,v=-\infty}^{\infty} \frac{1}{\left(u^2+v^2\right)^6} \equiv A_{12} = 4.06402 \quad .$$

The Coulomb potential for this crystal can also be computed. [3 points] Write down an expression for the Coulomb energy per lattice site of this structure. There is no need to simplify your expression, but be certain to define clearly all terms that you use.

[2 points] Describe in words how you would determine the equilibrium lattice parameter of the structure above given the Coulomb attraction and the repulsive part of the Lennard-Jones potential.

9. [10 points] The vacancy formation free energy at 300 K for Mo is approximately 2.3 eV. Compute the concentration of vacancies (i.e. number/cm^3) in Mo at room temperature. Mo forms a BCC crystal with cubic lattice parameter (at 3 00 K) of 3.14 Å. Boltzmann's constant is 8.61734×10^{-5} eV/K. You may assume that the concentration of vacancies is much less than the concentration of atomic sites.

10. In class, we studied the Kronig-Penney model for a 1-D crystal. Here we make reference to that discussion. Suppose that a 1-D "electron" is confined to a potential of that repeats periodically, and near the origin looks like:

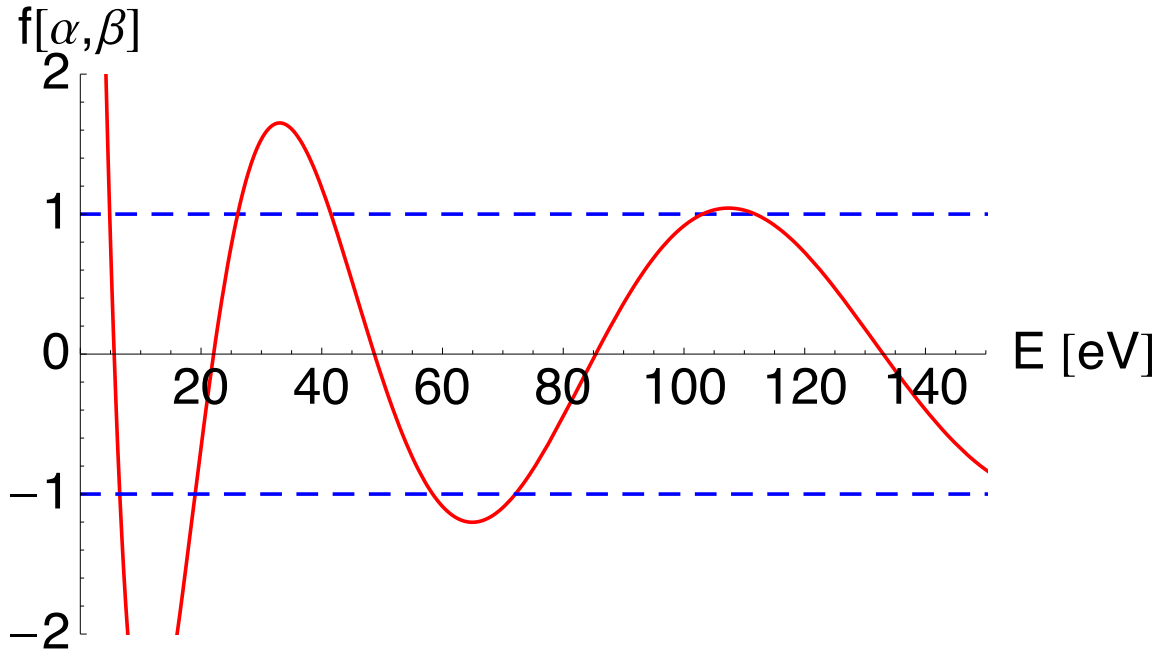


(a) [2 points] On the sketch above, draw on the x-axis (carefully!!) a primitive lattice vector, and label it **c**. Bloch's theorem places a constraint on the eigenfunctions of the Hamiltonian operator for an electron within this potential. [2 points] State one form of Bloch's theorem for this problem.

Continuing the analysis you started above, you eventually deduce that the following equation must hold:

$$\cos[(a+b)k] = \frac{1}{2\alpha\beta}(2\alpha\beta\cos[a\alpha]\cosh[b\beta] - \alpha^2\sin[a\alpha]\sinh[b\beta] + \beta^2\sin[a\alpha]\sinh[b\beta]).$$

Here, α and β depend on the energy, b is the width of the region in which the potential equals 50 eV, and a is the width of the regions for which the potential is equal to 0 eV. with E the energy of the electron, and k is the k appearing in Bloch's theorem. The plot below is a plot of the right hand side of this equation, defined to be $f[\alpha,\beta]$. [3 points] Indicate on the plot the values of E for which you expect to find a solution to the Schrödinger equation for this problem.



(c) Suppose that I tell you all accessible states below 107 eV are filled with two electrons, one spin up and one spin down. [1 point] Is the resulting one-dimensional material a metal or an insulator? [2 points] Explain your answer.