

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.

(1a) [10 POINTS] Suppose that the interaction between two atoms is given by the Lennard-Jones potential:

$$V(r) = 4\epsilon \left[\left(\frac{\sigma}{r} \right)^{12} - \left(\frac{\sigma}{r} \right)^6 \right] .$$

Consider a 2D crystal composed of these atoms with one atom per unit cell and primitive lattice vectors:

$$\mathbf{a} = \frac{\eta}{2} \mathbf{e}_1 + \frac{\eta}{4} \mathbf{e}_2$$

$$\mathbf{b} = \frac{\eta}{4} \mathbf{e}_1 - \frac{\eta}{2} \mathbf{e}_2$$

Define the energy per atom of this crystal to be:

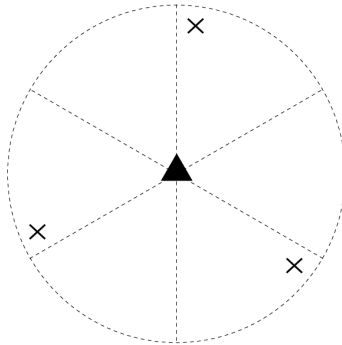
$$\frac{E}{atom} = 2\epsilon \left[A_{12} \left(\frac{\sigma}{\eta} \right)^{12} - A_6 \left(\frac{\sigma}{\eta} \right)^6 \right] .$$

Derive algebraic expressions for the constants A_{12} and A_6 .

(1b) [10 POINTS] Derive an expression for the value of η that minimizes the energy per atom of this 2D crystal in terms of the known quantities σ , ε , A_{12} and A_6 . Evaluate the total energy *per unit area* of the crystal at the equilibrium lattice parameter you calculated.

(2) [10 POINTS] Prove that if a 2nd rank tensor is symmetric in the unprimed frame, that it will be symmetric in the primed frame. Be certain to give a very clear explanation of the logic underlying your proof.

(3) A crystal has the point symmetry shown in the stereogram:



Use this symmetry to complete the rest of problem 3.

(3a) [10 POINTS] Consider two reference frames related by the symmetry operation 3. Assume that the axis of rotation coincides with \mathbf{e}_3 . Sketch the axes associated with the original reference frame, and those associated with the primed reference frame, and give the transformation matrix \mathbf{a} that transforms a vector from the original frame to the primed frame.

(3b) [10 POINTS] Using the matrix \mathbf{a} constructed above, derive expressions for σ'_{11} and σ'_{12} in terms of σ_{11} , σ_{22} , and σ_{12} , where the σ_{ij} 's are elements of the symmetric conductivity tensor.

(3c) [5 POINTS] Based on the expressions you derived in part (b), derive constraints on the values of σ_{11} , σ_{22} , and σ_{12} in this material.

(4) [10 POINTS] A cubic material is distorted according to the following *distortion tensor*:

$$\mathbf{e} = \begin{bmatrix} \alpha & \gamma & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

Give the associated stress tensor in terms of the parameters α and γ and the elastic constants C_{11} , C_{12} and C_{44} . Recall that the strain tensor is the symmetric part of the distortion tensor. Also, recall that in Voigt notation, the index pairs ij map onto the single indices n according to:

ij	11	22	33	23 or 32	13 or 31	12 or 21
n	1	2	3	4	5	6

Finally, recall that the elastic constant matrix for cubic materials is given by:

$$\mathbf{C} = \begin{pmatrix} C_{11} & C_{12} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{11} & C_{12} & 0 & 0 & 0 \\ C_{12} & C_{12} & C_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & C_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & C_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & C_{44} \end{pmatrix}.$$

(5) An electron bound to a hydrogen atom is described by the wavefunction:

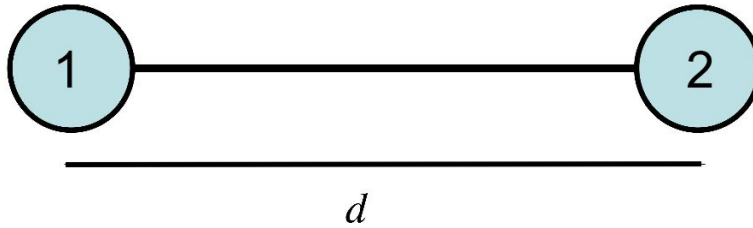
$$\Psi(\mathbf{r}, t) = \frac{1}{\sqrt{3}} \exp\left(\frac{-iE_4 t}{\hbar}\right) \psi_{420}(\mathbf{r}) - i\sqrt{\frac{2}{3}} \exp\left(\frac{-iE_2 t}{\hbar}\right) \psi_{21-1}(\mathbf{r}),$$

with $\psi_{nlm}(\mathbf{r})$ an eigenfunction of the Hamiltonian operator of the H atom, \hat{H} , squared angular momentum operator, \hat{L}^2 , and z-component of the angular momentum operator, \hat{L}_z .

(5a) [5 POINTS] Give the expectation value of the total energy.

(5b) [5 POINTS] Give the expectation value of the z-component of the angular momentum, \hat{L}_z , for the electron.

(5c) [5 POINTS] Give the expectation value of the angular momentum squared, \hat{L}^2 .



(6) Suppose that we consider the formation of a bond between a H^- and a neutral H atom (so there are three electrons in total – initially one atom has two electrons in its ground state with energy E_o , and the other has one electron, initially in the ground state with energy E_o). Assume that you write the eigenfunction of the molecule as a linear combination of the ground state eigenfunctions of the bare atoms:

$$\psi_{mol}(\mathbf{r}) = b_1\psi_1(\mathbf{r}) + b_2\psi_2(\mathbf{r}),$$

with $\psi_1(\mathbf{r})$ the eigenfunction of the bare H atom on the left, and $\psi_2(\mathbf{r})$ the eigenfunction on the right H atom. (Note that the states $\psi_1(\mathbf{r})$ and $\psi_2(\mathbf{r})$ are real.) Assume further that

$$\int d\mathbf{r} \psi_i(\mathbf{r})\psi_j(\mathbf{r}) = \delta_{ij}.$$

Within this basis, the Hamiltonian matrix, \mathbf{H} , is given by:

$$\mathbf{H} = \begin{pmatrix} \int d\mathbf{r} \psi_1(\mathbf{r}) \hat{H} \psi_1(\mathbf{r}) & \int d\mathbf{r} \psi_1(\mathbf{r}) \hat{H} \psi_2(\mathbf{r}) \\ \int d\mathbf{r} \psi_2(\mathbf{r}) \hat{H} \psi_1(\mathbf{r}) & \int d\mathbf{r} \psi_2(\mathbf{r}) \hat{H} \psi_2(\mathbf{r}) \end{pmatrix} = \begin{pmatrix} E_o & -\frac{V_o}{d} \\ -\frac{V_o}{d} & E_o \end{pmatrix},$$

with V_o a positive number, and d the distance between the nuclei.

(a) [5 points] What possible energies might one measure for an electron bound to the dimer with bond length d ?

(b) [5 points] Give the coefficients b_1 and b_2 for the antibonding state, and state how these are related to the Hamiltonian matrix, \mathbf{H} . Sketch the values of the antibonding state of the molecule along the straight line passing through the nuclei of the atoms.

(c) [5 points] Calculate the change in electronic energy upon forming the dimer with a bond length d .

(d) [5 points] Now suppose that in addition to the change in electronic energy, there is a repulsive energy that depends on the separation of the nuclei according to:

$$E_{rep}(d) = \frac{A}{d^4},$$

with A a positive constant. Given this repulsive energy, and the change in electron energy you computed in part (c), give the equilibrium bond length of the H_2^- molecule in terms of A and V_o .