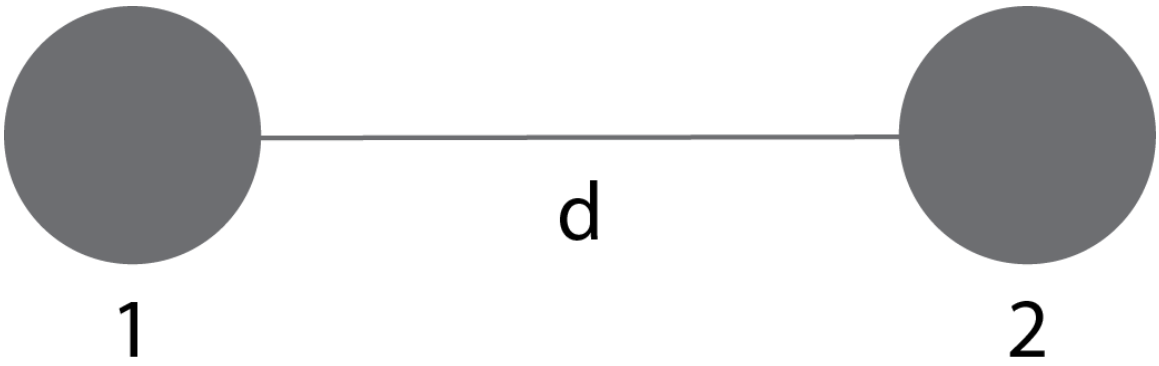
MSE 102, Fall 2014 Midterm #2

Write your name here [10 points]: _____

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 may use a calculator.
- You should circle your answer. You should also complete this exam in pen.
- There are a total of 110 points (including the 10 above for writing your name). 100 points will be considered a perfect score. Remaining points will be used as extra credit.
- Feel free to ask questions, but only for clarification purposes.



1. We can use our understanding of quantum mechanics to model bonding of atoms in a 1-dimensional world. Suppose that the molecule in the figure above is composed of two atoms – both 1-dimensional hydrogen atoms. Assume that the eigenfunctions for the electrons bound to the bare atoms are given by:

$$\psi_1(x) = \exp(-|x|)$$
$$\psi_2(x) = \exp(-|x-d|)$$

We will use these states as a basis.

(a) **[5 points]** Are these states properly normalized? You *must* justify for your answer with a direct and correct calculation. Note that these states are identical, just defined about a different origin.

(b) **[5 points]** Are these states orthogonal? Again, you *must* justify your answer with a direct, and correct calculation.

In what follows, we will assume that the states $\psi_1(x)$ and $\psi_2(x)$ are orthonormal. The matrix elements for the Hamiltonian operator of the molecule are defined to be:

$$\int_{-\infty}^{\infty} dx \psi_1^*(x) \hat{H} \psi_1(x) = E_o$$

$$\int_{-\infty}^{\infty} dx \psi_2^*(x) \hat{H} \psi_2(x) = E_o \qquad .$$

$$\int_{-\infty}^{\infty} dx \psi_1^*(x) \hat{H} \psi_2(x) = -\frac{A^2}{d^2+4}$$

(c) **[10 points]** Construct the Hamiltonian matrix for the molecule, and compute its eigenvalues and eigenvectors. Sketch the eigenfunction of the antibonding state, and describe in words its important features. (That is, explain why we call this the antibonding state?)

Now suppose that the molecule has three electrons. Moreover, assume that the repulsive interaction between the nuclei is given by:

$$V_{rep}(d) = \left(\frac{B}{d}\right)^2 \quad .$$

(d) **[10 points]** Find the equilibrium bond length for the molecule in terms of the parameters A and B. Assume that A and B are both real, and that $A > B > 0$.

2. **[10 points]** In class, we discussed the meaning of Hermitian operators. These operators are important to us, because as you know, these operators have real eigenvalues. More specifically, an operator $\hat{A}$ is Hermitian if

$$\int dx(\hat{A}^{\dagger}\psi^{*}(x))\phi(x) = \int dx\psi^{*}(x)\hat{A}\phi(x) \quad \forall \quad \psi(x),\phi(x) \text{ in the Hilbert space.}$$

Consider the operator

$$\hat{A} = -i\hbar x\frac{d}{dx} \ .$$

Is this operator Hermitian? Again, justify your answer with a rigorous mathematical argument.

3. When noble gases condense on a surface, they can be considered to form a 2-D crystal. This crystal can be described quite well using a Lennard Jones potential:

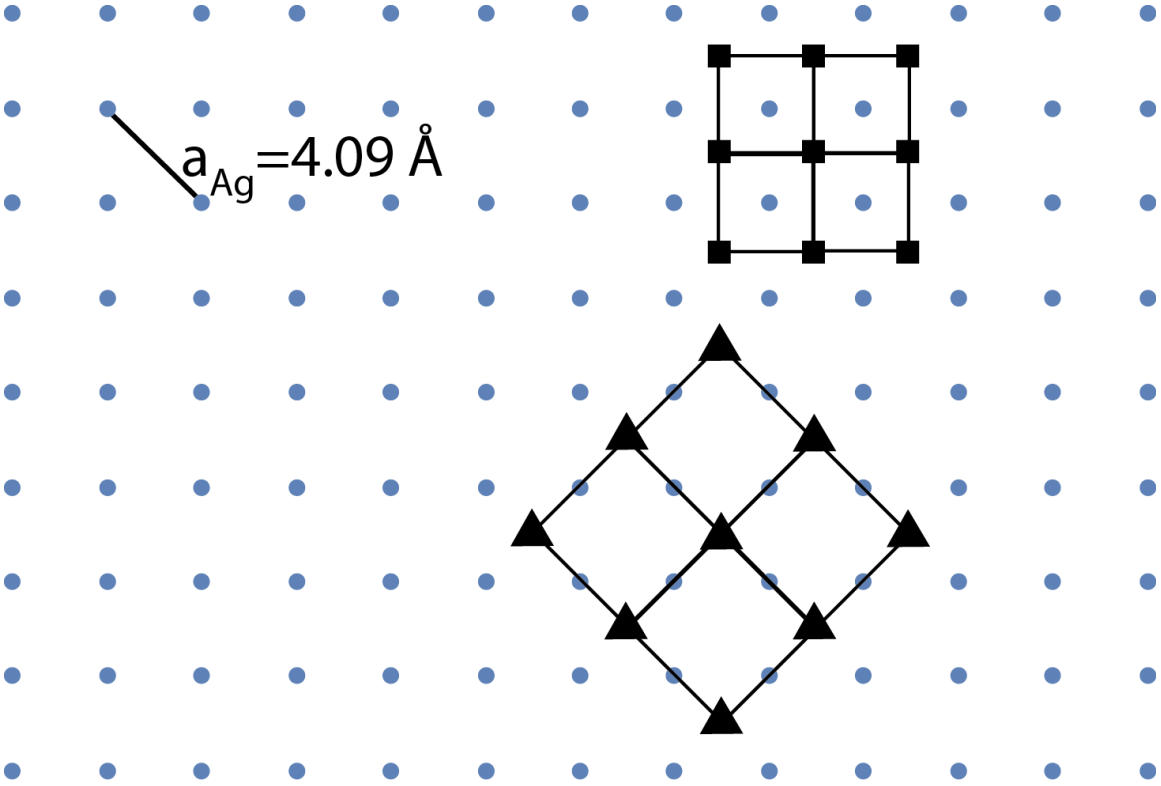
$$V(r) = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right] \quad .$$

(a) **[10 points]** *Derive* the equilibrium bond length, and the energy per atom of a one atom per unit cell crystal defined on a simple square lattice (in 2-D) with square edge of length a. You should express your answers algebraically in terms of the constants σ, ε, and the parameters A_{12} and A_6 we defined in class. Compute numerically the energy per atom of the crystal at its equilibrium lattice parameter in terms of the parameter ε. You may need the sums:

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

$$A_6 \equiv \sum_{u=-\infty}^{\infty}\sum_{v=-\infty}^{\infty}\frac{1}{\left(u^2+v^2\right)^3} = 4.65891$$

(b) **[10 points]** Now assume that Kr gas is deposited on the (001) surface of a Ag crystal (Ag is an face centered crystal with cubic lattice parameter $a = 4.09$ Å. The structure of this surface is shown in the figure below. Consider the two arrangements of Kr atoms indicated by the triangles and the squares. Suppose that Kr atoms remain on the surface, and they have a minimum energy when sitting at the interstitial gaps in the surface, as shown below. Assume that the only other contribution to the energy is the Lennard-Jones interaction between the Kr atoms. Given that the value of σ for Kr is known to be $\sigma_{Kr} = 3.684$ Å, which of these structures do you expect to find experimentally? Justify your response through a calculation of the energy per atom of each configuration. Note that in the definition of the Lennard-Jones potential, the parameter $\varepsilon > 0$.



4. There is an electron confined to the $\mathbf{e}_1$ axis. The potential energy is defined by $V(x)=0$ for all $0 \le x \le L$ and infinite for all other x.

(a) **[5 points]** Suppose the wavefunction of the electron is $\Psi(x,t)$. What are the values for $\Psi(0,t)$ and $\Psi(L,t)$. Explain your answer.

(b) **[5 points]** The eigenfunctions inside the box have the form:

$$\psi_n(x)=\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right), n=1,2,3,\cdots$$

Plug this into the time-independent Schrodinger equation and find the energy eigenvalue associated with $\psi_n(x)$.

(c) **[5 points]** Suppose the wavefunction of the electron can be written at time $t = 0$:

$$\Psi(x, t=0) = \exp\left(-i\frac{\pi}{5}\right)\sqrt{\frac{2}{L}}\sin\left(\frac{\pi}{L}x\right) + C\sqrt{\frac{2}{L}}\sin\left(\frac{3\pi}{L}x\right)$$

Give a value of constant C that satisfies the normalization condition.

(d) **[5 points]** Further calculate the energy expectation value for the state you identified in part (c).

5. **[20 points]** Gold crystallizes in an FCC structure (that is a cubic F-lattice with one atom per primitive unit cell). A crystal of gold is placed under a hydrostatic pressure P such that the stress tensor is given by:

$$\underset{\approx}{\sigma} = \frac{1}{3}\begin{bmatrix} -P & 0 & 0 \\ 0 & -P & 0 \\ 0 & 0 & -P \end{bmatrix}.$$

Compute the elastic energy per atom of the crystal in terms of the parameter P and the cubic lattice parameter of gold, a_o. 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

and that the elastic constant matrix for cubic materials is given by:

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