1. Solving problems is momentum space. (20 points)

In the position-space representation of quantum mechanics, we use a spatial and time dependent wave function and a group of operators for position and momentum to determine the expectation values of various ensemble measurements.

Recently, we have been discussing the momentum space representation, where the wave functions are functions of MOMENTUM and time, and there are new representations of the position and momentum operator. The goal in this problem is to see how this new representation works, and come to see that it really is a general and alternative way to do quantum mechanics.

a) In class, we demonstrated that the momentum operator is just multiplication by the numerical value of momentum: \( \hat{p} = p \) in this representation. I asserted in class that \( \hat{x} = i\hbar \frac{d}{dp} \). Prove that it works by showing that the expectation value of position in the momentum representation:

\[
\langle x \rangle = \int_{-\infty}^{\infty} dp \phi^*(p) i\hbar \frac{d}{dp} \phi(p)
\]

can be reduced to our old friend, the expectation value of position in the position representation. [5 points]

b) Show in this representation what the value is for \([x, p]\). Look familiar? [5 points]

c) Now that you know the operators in this representation, you can write down the harmonic oscillator Hamiltonian in the momentum representation. Do so and you'll have a second order differential equation in momentum derivatives. See if you can solve this equation: Use some collection of constants and define a dimensionless momentum and a dimensionless energy. In terms of dimensionless momentum and energy, what is the Schrödinger Equation now? What is the behavior for very large momentum? Use that behavior to guess a form for the solutions. Use a series solution. Explain quickly why the series needs to terminate. What does termination of the series force the eigen energies to be?? What is the lowest energy and the associated lowest momentum wave function? Show via the Fourier Transform that you have also found exactly the same state that we found using the spatial representation. [10 points]
2. **The double potential well as a model for diatomic molecules.** (30 points)

At this point in the course, we have been studying special cases long enough that you might start to feel that we’ve lost touch with our goal, namely, to understand the behavior of real systems. Let’s take what we’ve learned about piece-wise potentials and see whether we can begin to understand some of the behavior of diatomic molecules. REAL diatomic molecules, even the simplest case, H$_2$, involve multiple particles, so we will need to make a few statements about such systems near the end in order to generalize to reality. Still, this exercise provided the early pioneers of quantum physics with enough insight about chemical bonding so that the simple double well, applied artistically, still forms the basis of our understanding.

In this problem, our goal is to understand why it might be energetically favorable for isolated atoms to share electrons. Since diatomic molecules are reflection symmetric, we will use a 1-d symmetric double well potential.

a) **The isolated atomic wells.** For atomic problems, the Schrödinger Equation involves the Coulomb potential of interaction between the negatively charged electrons and the positive nucleus (and the similar repulsive Coulomb terms between all the various electrons, which makes the problem intractable except for hydrogen!). This potential is defined to be equal to zero at infinite distance. Therefore, to simulate the Coulomb potential, let’s define atomic wells that are zero outside the well, and negative (attractive) inside the well. Give each atom a well of width, $a$, and depth $-V_0$. Further, we will concentrate on the outer-most electrons in the atom, the valence electrons, and assume that somehow all the other electrons plus the nucleus help to create the potential well that holds the valence electrons.

As you know, the typical atom is a few angstroms ($10^{-10}$ meters) across and the valence electrons require an energy of a few electron volts to remove them (for example, that’s the size of the work function for metals in the photoelectric effect). We need to see whether our potential well at least gives us the flavor of atomic physics. So, let’s see how the numbers work out:

Calculate how deep the square potential of width 0.2 nm must be, so that we have at least two bound states for electrons in the well. (5 points)

b) **Total electronic energy of the isolated atoms.** Now imagine that we have two atoms and that each of them has a single valence electron. Assume that each atom is like the situation above, so that there are just barely two possible bound states in each well. Assume that there is an electron in the ground state of each well. Assume that the atoms are so far apart that you can calculate the energy of each electron ground state as though the other well was not even there (isolated atoms). For that isolated case, write down the transcendental equation that you must solve to determine the energy of an electron in the atomic well. Then solve the equation for each electron. Finally and calculate the TOTAL electronic energy of this
system (Remember!! You have two atoms, so add up all the energy) Be sure that 
you include the sum of both KE and PE for both electrons.

You will need to solve the transcendental equation for the ground state energy in 
the well. Mathematica is pretty good at finding numerical roots, but many of your 
graphing calculators can do it too.

You now have the total valence electronic energy of the isolated atoms. (5 points)

c) The final molecule. Now assume that the two atoms just touch, so that they create 
a single potential well that is TWICE the width, but remains at the same depth. 
Write down the transcendental equation that you need to solve for the energies 
now. How many states are allowed in this new well? Calculate the total 
electronic energy for this well, assuming that the two electrons share the ground 
state (true in real molecules because the have opposite spin, so the Pauli Principle 
let’s them coexist in the same ground state). (5 points)

d) Insight. With any luck, in part (c) you will have found a decreased total energy 
for this case. We have various contributions to the total energy, two potential 
terms and two kinetic terms. When you look at your final result, which terms 
have caused the energy to go down?? Now use your physical insight and an 
argument based on the Uncertainty Principle to make a simple statement of how 
the final energy SHOULD HAVE BEHAVED when going from isolated atoms to 
the final diatomic molecule. (5 points)

e) Why stop at just touching? Suppose that the two atoms continue to merge 
together and that the main effect is that the total well decreases in width. You 
might think that the well should get deeper too. Make an argument based on the 
combination of electron-nucleus attraction compared with electron-electron 
repulsion that suggests it might or might not..., and assume that the well stays the 
same depth. If the atoms were to totally overlap, the final well would be the 
original depth, but of the original width. Do you agree with or disagree with the 
following statement?

“Overlap between the wells is clearly an net benefit energetically as the smaller 
potential well width clearly causes the total electronic energy to decrease. The 
atoms in this model will prefer to be totally overlapped.” Explain your position 
clearly. (10 points).