

In this lab we will play around with covalent bonds. In class we considered an particle in a double square well potential. By symmetry, we expect the probability function  $\Psi^*\Psi$  in one of the wells to be the mirror reflection of the other well. When the wells are far apart, the wave function decays almost to zero in between the wells, and the energy eigenstate wave functions in each well look pretty much like they would if the other well were not present. But for each energy of a single square well potential, there are two states in the well-separated double well. With the wave function decaying to such a small level between the wells, it doesn't cost much energy to make a node precisely between the two wells. Putting in this node changes the wave function from one which curves upward in both wells to one which curves upward in one and downward in the other.

As the wells get closer together, two things happen. First of all, the states which don't have a node between the wells don't decay so close to zero anymore. This results in longer wavelengths and lower energies. If the energy goes down when they get closer, that implies a force pushing them together (because force is just minus the gradient of potential energy). The second thing that happens is that the energy cost for putting a node between the two wells goes up. This means that the energy of the eigenstates with a node between the wells goes up as the wells get closer, implying a force which pushes the wells apart.

Start up the program, and enter 100 for "mass/hbar^2" and `-squarepulse(5*x)` for the "Potential: V(x)." Now click on "recaluculate" and look at the wave functions and energies which the program calculates for the  $n = 0$  and  $n = 1$  states. Write the energies in the space provided below. (You have to click on "recaluculate" any time you change  $m$  or  $V(x)$ , but not when you change  $n$ .)

$$E_{n=0} = \underline{\hspace{2cm}} \quad E_{n=1} = \underline{\hspace{2cm}}$$

Now change the potential to `-(squarepulse(5*(x+a/2))+squarepulse(5*(x-a/2)))` where **a** is any number you want. The parameter **a** represents the spacing between the centers of the two wells. Enter the following values for **a** in the table below, and record the energy of the lowest four energy eigenstates.

<b>a</b>	$E_{n=0}$	$E_{n=1}$	$E_{n=2}$	$E_{n=3}$
1	<u>                    </u>	<u>                    </u>	<u>                    </u>	<u>                    </u>
0.6	<u>                    </u>	<u>                    </u>	<u>                    </u>	<u>                    </u>
0.5	<u>                    </u>	<u>                    </u>	<u>                    </u>	<u>                    </u>
0.4	<u>                    </u>	<u>                    </u>	<u>                    </u>	<u>                    </u>

Which of the four states result in attraction? \_\_\_\_\_ Which states result in repulsion? \_\_\_\_\_