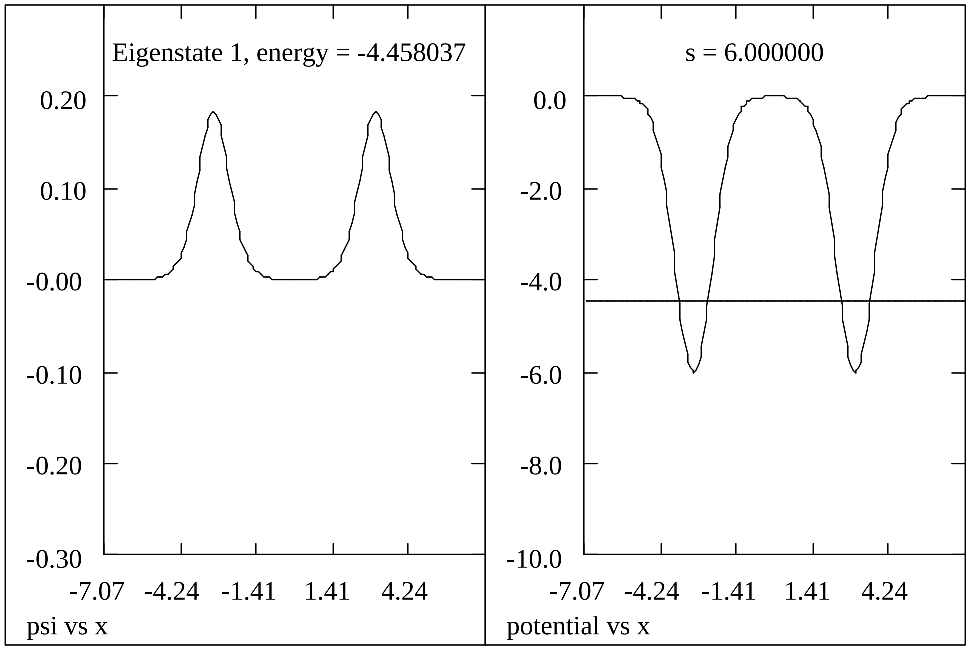

Figure 1: Ground state wave function and energy for the symmetric double well problem with well separation $s = 6$.

1 Double Potential Well and Degeneracy

In this section a bound state problem consisting of two potential wells is solved using the finite matrix approximation. The wells are Gaussian in shape and have a separation of s. The potential has the form

$$U(x) = -6[\exp\{-(x - s/2)^2\} + \exp\{-(x + s/2)^2\}] \tag{1}$$

and the resulting Hamiltonian is

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} + U(x). \tag{2}$$

Using the RLaB demonstration program *dwell_demo.r*, we can find the wave functions and energies for the first two bound states. Figure 1 shows that the lowest energy state wave function is symmetric about $x = 0$ and thus has parity $P = 1$. On the other hand, the first excited state wave function has parity $P = -1$. However, notice that the two states differ in energy by

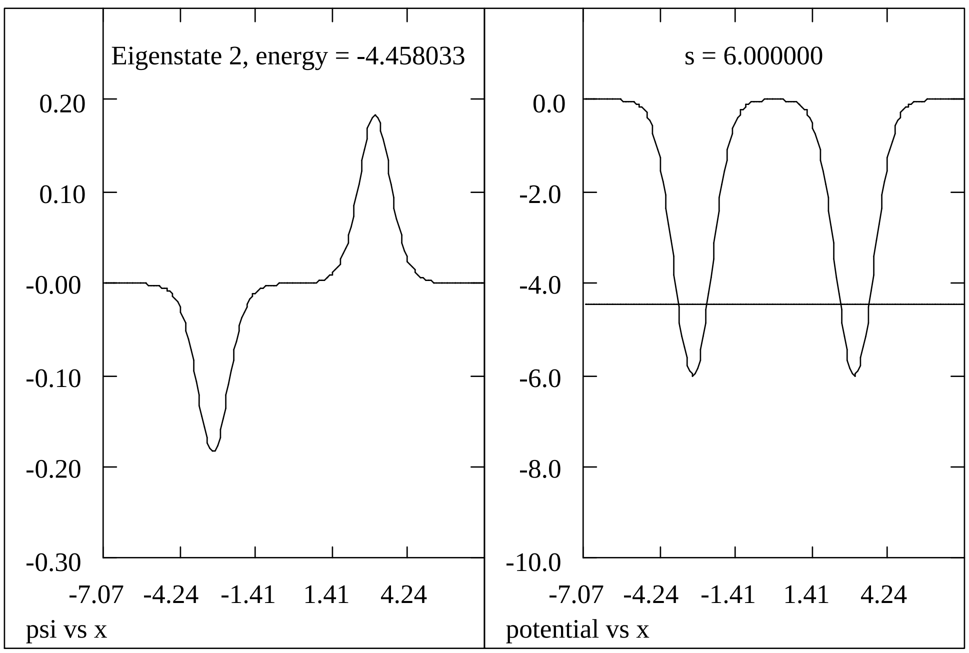

Figure 2: First excited state wave function and energy for the symmetric double well problem with well separation $s = 6$.

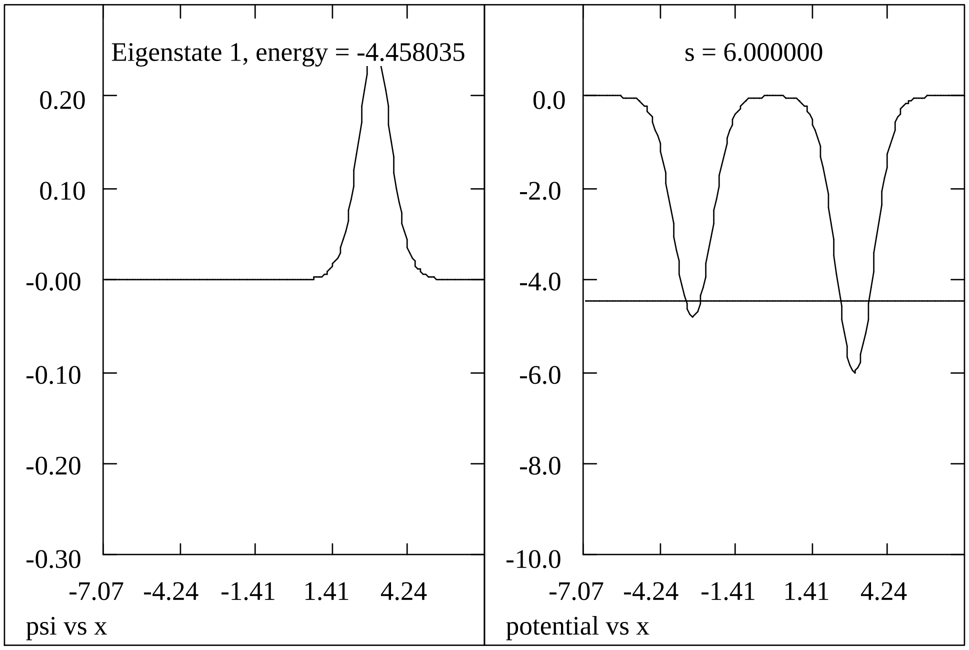

Figure 3: Ground state wave function and energy for the asymmetric double well problem with well separation $s = 6$.

only a tiny amount — in other words, the Hamiltonian for this problem is almost degenerate for the first two eigenvectors. Why is this so?

Examination of figures 1 and 2 shows that the wave function decays almost to zero in the interval between the potential wells. To a very good approximation we can think of this problem as two separate problems, namely, obtaining the wave function and eigenvalue for a potential in the region $x < 0$, and doing the same for another potential in the region $x > 0$. Since in each case the wave functions become very small in the region near $x = 0$, these two problems may be solved independently. The actual solutions that we see are linear superpositions of the two independent solutions, the first being the left plus the right solution, the second being the left minus the right solution.

The fact that the energies for the two solutions shown in figures 1 and 2 aren't *exactly* equal is a consequence of the slight effect of each potential on the tail of the wave function associated with the other potential. The true eigenvectors in this case are thus the definite parity states illustrated in these figures.

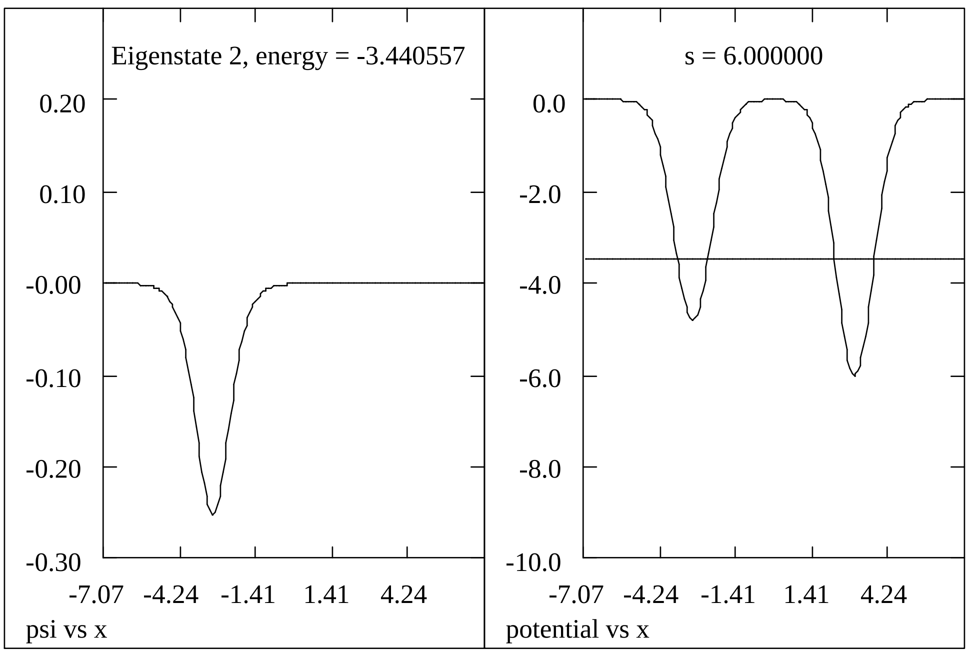

Figure 4: First excited state wave function and energy for the asymmetric double well problem with well separation $s = 6$.

A very different result occurs when the potentials are not of the same depth (see *adwell_demo.r*). Figures 3 and 4 show the ground and first excited states for a case in which the left potential well is 20% weaker than the right well. In this case the ground state solution is clearly associated with the stronger potential well on the right, while the first excited state is associated with the weaker left potential. Since the aggregate potential function is not symmetric with respect to $x = 0$, the parity operator no longer commutes with the Hamiltonian and energy eigenstates are no longer parity eigenstates. Thus, symmetry or antisymmetry of the wave function is no longer forced by the parity operator. The ground state solution is very close to being a solution for the right potential well alone, and the first excited state is nearly a solution for the left potential well by itself. However, the energies for these two solutions are now very different, and a superposition of these two eigenstates is not even approximately an eigenstate of the Hamiltonian.