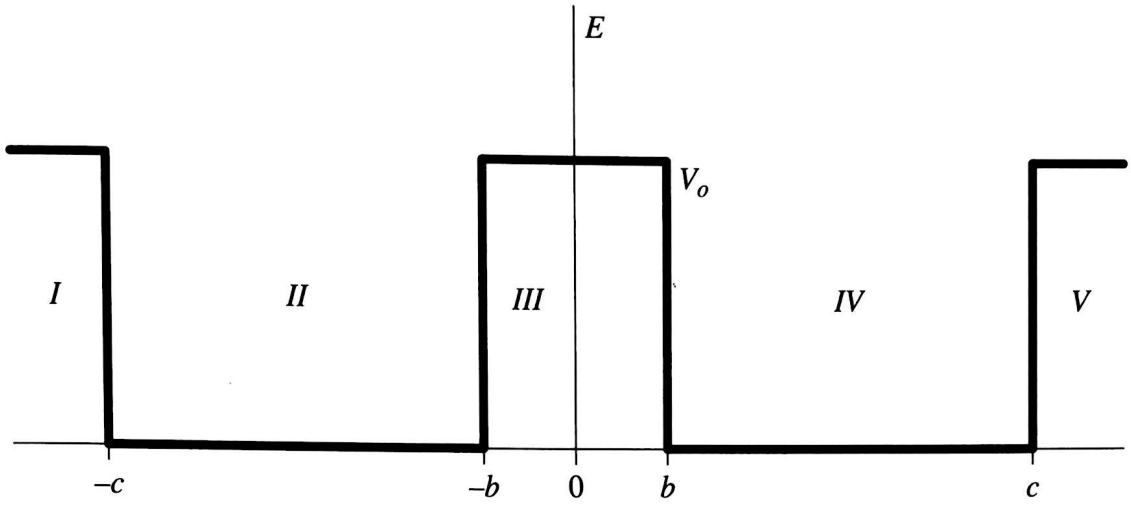

Figure 2.10 The double square well.

From physical reasoning, how must the lowest eigenvalues and their wavefunctions behave in the limit that the distance between the wells vanishes?

2.13 The Propagator Method

Before addressing the double square well problem, let's develop an alternate approach to the single well problem, based on the concept of a *propagator*. First, let's revisit the single well.

Let's assume that we have the solution $\Psi(b)$ and its derivative $\Psi'(b)$ at the left side of the well, $x = b$. The region between b and c is a classically allowed region, so in this region the solution is just

$$\Psi = A\sin(\alpha x) + B\cos(\alpha x) \tag{2.93}$$

and hence

$$\Psi' = A\alpha\cos(\alpha x) - B\alpha\sin(\alpha x). \tag{2.94}$$

Requiring this solution to match the known values of Ψ and Ψ' at b yields two equations that we can solve for the unknown values of A and B:

$$A = \sin(\alpha b)\Psi(b) + \frac{1}{\alpha}\cos(\alpha b)\Psi'(b),$$

$$B = \cos(\alpha b)\Psi(b) - \frac{1}{\alpha}\sin(\alpha b)\Psi'(b). \tag{2.95}$$

This doesn't look particularly appealing, and it's going to get worse before it gets better! Substituting these expressions for A and B into Equation 2.93 for $\Psi(x)$,

we find

$$\begin{aligned}\Psi(x) &= \left(\sin(\alpha b)\Psi(b) + \frac{1}{\alpha}\cos(\alpha b)\Psi'(b)\right)\sin(\alpha x) \\ &\quad + \left(\cos(\alpha b)\Psi(b) - \frac{1}{\alpha}\sin(\alpha b)\Psi'(b)\right)\cos(\alpha x) \\ &= \big(\sin(\alpha b)\sin(\alpha x) + \cos(\alpha b)\cos(\alpha x)\big)\Psi(b) \\ &\quad + \frac{1}{\alpha}\big(\cos(\alpha b)\sin(\alpha x) - \sin(\alpha b)\cos(\alpha x)\big)\Psi'(b) \\ &= \cos[\alpha(x-b)]\,\Psi(b) + \frac{1}{\alpha}\sin[\alpha(x-b)]\,\Psi'(b), \end{aligned} \tag{2.96}$$

and for the derivative we find

$$\Psi'(x) = -\alpha\sin[\alpha(x-b)]\,\Psi(b) + \cos[\alpha(x-b)]\,\Psi'(b). \tag{2.97}$$

This is certainly simpler than what we had, but it takes on even greater elegance when we write it in matrix form,

$$\begin{aligned}\begin{bmatrix}\Psi(x)\\ \Psi'(x)\end{bmatrix} &= \begin{bmatrix}\cos[\alpha(x-b)] & \frac{1}{\alpha}\sin[\alpha(x-b)]\\ -\alpha\sin[\alpha(x-b)] & \cos[\alpha(x-b)]\end{bmatrix}\begin{bmatrix}\Psi(b)\\ \Psi'(b)\end{bmatrix} \\ &= P_{allowed}\begin{bmatrix}\Psi(b)\\ \Psi'(b)\end{bmatrix}, \end{aligned} \tag{2.98}$$

where

$$P_{allowed} = \begin{bmatrix}\cos[\alpha(x-b)] & \frac{1}{\alpha}\sin[\alpha(x-b)]\\ -\alpha\sin[\alpha(x-b)] & \cos[\alpha(x-b)]\end{bmatrix}. \tag{2.99}$$

It's in this form that we see the matrix "propagating" the solution from b to x. That is, the "solution" (both Ψ and Ψ') is "propagated," or carried forward, from b to x by this matrix multiplication. It's also noteworthy that the propagation matrix depends only upon the distance $x - b$, and not on x or b themselves.

At this point, we're ready to solve our problem. There are several different ways we could proceed; for example, we could place the potential symmetrically about the origin, thus taking full advantage of the symmetry of the problem. We would then propagate the solution from $-\infty$ up to 0 and require that $\Psi'(0) = 0$ for the even states, and $\Psi(0) = 0$ for the odd states. A problem's symmetry can often be used in this way to simplify the solution, but it isn't *necessary*. We'll demonstrate this by developing a method that doesn't utilize the symmetry of the problem—but in so doing our solutions will no longer naturally fall into an even/odd category.

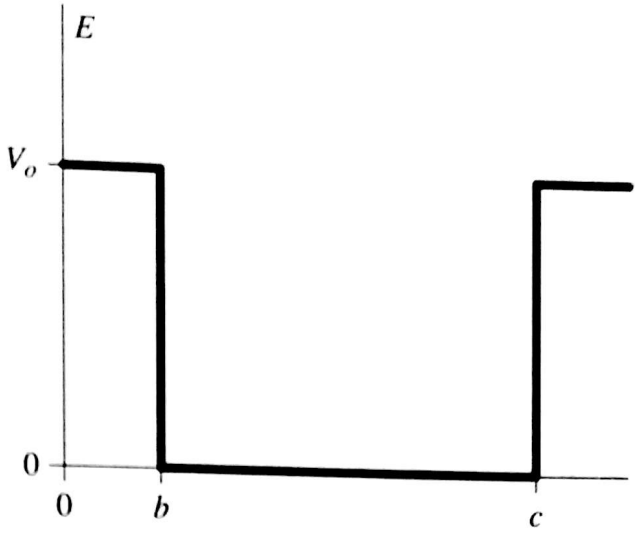

Figure 2.11 Another single well.

Let's begin in the region left of the well in Figure 2.11, $x < b$. In this region we know that the solution must be

$$\Psi(x) = Ge^{\beta x} \tag{2.100}$$

so that

$$\Psi'(x) = G\beta e^{\beta x}. \tag{2.101}$$

The overall normalization isn't important; what *is* important is the relationship between Ψ and Ψ', namely that

$$\Psi'(x) = \beta\,\Psi(x), \qquad x < b. \tag{2.102}$$

From continuity, this must be true at $x = b$ as well. Computationally, we can choose any nonzero value for Ψ—let's choose $\Psi(b) = 1$, and Equation 2.102 gives $\Psi'(b) = \beta$. We then propagate the solution (and its derivative) from b to c, using the free propagator of Equation 2.98.

For $x > c$, we know the solution is exponentially decaying,

$$\Psi(x) = Ge^{-\beta x}, \tag{2.103}$$

so that

$$\Psi'(x) = -G\beta e^{-\beta x} \tag{2.104}$$

and

$$\Psi'(x) = -\beta\,\Psi(x), \qquad x > c. \tag{2.105}$$

The matching condition at $x = c$ that the acceptable wavefunction must satisfy is then

$$\Psi'(c) = -\beta\,\Psi(c) \tag{2.106}$$

where $\Psi(c)$ and $\Psi'(c)$ were evaluated by propagation. The function whose roo we're seeking is then simply

$$f(E) = \Psi'(c) + \beta\,\Psi(c), \tag{2.1}$$

and those roots are then the eigenvalues of the well. Note that since we did no invoke symmetry in deriving this expression, the parity of the solution doesn't en in.

EXERCISE 2.16
Verify that this propagator approach leads to exactly the same solutions for th square well as obtained earlier.

2.14 The Double Well

Now consider a system composed of two wells, separated by some distance, as Figure 2.12. If this distance is large, then the wells are isolated and the allowe energies of the system are the same as for a single well. But if the distance is n too large the wavefunction of one well can penetrate the barrier into the other we so that the two wells interact. A major advantage of the propagator approach that it is easily applied to this case, with virtually no increase in difficulty, while t "matching boundary conditions" approach leads to greater and greater complexi (Note, of course, that these two approaches are actually the same, it's just that t algebra has been rearranged to *appear* less complicated.)

We already know how to propagate the solution in the allowed region. The a propriate propagator for the forbidden region can be derived in exactly the sa manner.

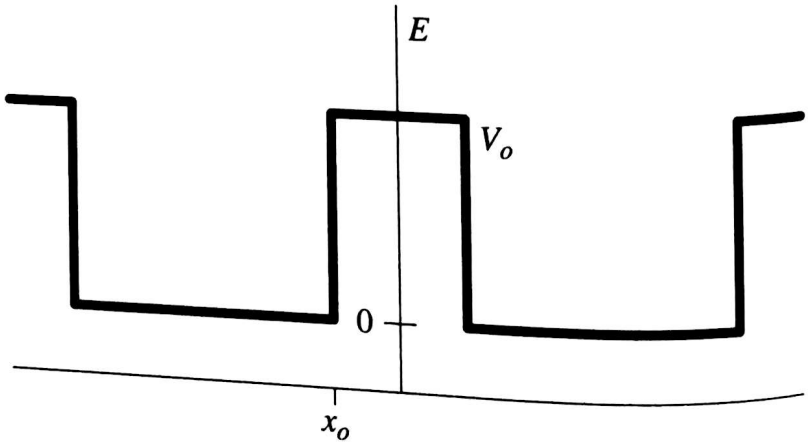

Figure 2.12 A double well

EXERCISE 2.17

Show that the propagator for the forbidden region is

$$P_{forbidden} = \begin{bmatrix} \cosh[\beta(x - x_o)] & \frac{1}{\beta}\sinh[\beta(x - x_o)] \\ \beta\sinh[\beta(x - x_o)] & \cosh[\beta(x - x_o)] \end{bmatrix}. \tag{2.108}$$

The procedure for propagating the wavefunction should be clear: as before, start in the forbidden region to the left of all wells. If the wells are identical, we can use the symmetry of the problem to cut the work somewhat. With the propagator for the allowed region, find the wavefunction (and its derivative) across the first well, and then propagate with the forbidden region propagator to the origin, where the parity of the wavefunction is used to determine if the wavefunction or its derivative should be zero. If the wells are not identical, propagate through the allowed region, all the way through the forbidden region, and then through the second allowed region, matching up with the known behavior at the right side of the second well.

EXERCISE 2.18

Solve for all the energies of the double well, with $V_o = 10\,\text{eV}$ and the well width, W, being 0.6 nm as before. (Our earlier a was half the well width.) Let the separation between the wells, S, be 0.2 nm. Then vary the distance between the wells, and plot the lowest two energies of the system versus separation distance.

2.15 A One-Dimensional Crystal

As we add more wells to our problem, as indicated in Figure 2.13, we are in fact developing a one-dimensional model of a crystal. Imagine that we're interested in a model having N identical wells of width W, separated by the same barrier width S.

Starting at the far left, we have a sequence of a well followed by a barrier, repeated N times. The solution can be propagated through this system of wells

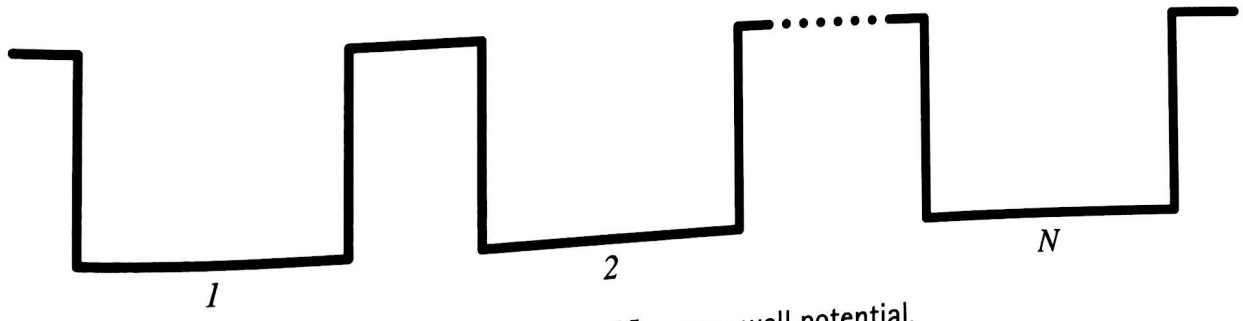

Figure 2.13 The N-square well potential.

and barriers, and finally matched with the exponentially decaying solution at the far right. Alternatively, we could place the origin at the geometric center, integrate up to the origin, and apply parity restrictions to determine the eigenvalues.

The only remaining difficulty lies with the "global" search strategy. The energy levels of the single well are separated by many eV, so that a 0.1 eV search region was sufficiently small. But with the multiple well system, we're seeing a splitting of the energy levels, and this splitting is much smaller than the difference between the basic energy levels. For the double well, this splitting was on the order of 0.1 eV— since the two states were of opposite parity, we didn't have a problem. But with the many well system, we might. To be "safe," let's choose the search increment to be $0.1/N$, for a system of N wells.

EXERCISE 2.19

Modify your code to treat this many well problem. Use your program to investigate the energy structure of the model crystal with increasing N. What can you say about the limit as $N \to \infty$?

2.16 A Note on *Fast* Algorithms

When investigating an N well problem, it would seem that we would need to perform (on the order of) N matrix multiplications. But this is not the case. In fact, to multiply N identical matrices, all we need is (on the order of) $\ln(N)$ multiplications! (In this discussion, we take the matrix A to be the propagator from the left of one well to the left of the next well, e.g., the product of the propagators for allowed and forbidden regions.)

Consider the expression

$$B = A \times A \times A \ldots A \times A.$$

By evaluating $A^2 = A \times A$, we can evaluate B as

$$B = A^2 \times A^2 \cdots \times A^2$$

and cut in half the number of required multiplications. Evaluating $A^4 = A^2 \times A^2$, we reduce the total another factor of two, and so on. If $N = 2^m$, then instead of $N - 1$ multiplications, B can be evaluated with $m - 1$ multiplications.

This reduction by repeated halving of the effort is the essence of so-called *fast algorithms,* the best known of which is the *Fast Fourier Transform,* which we'll investigate later.