5

A Particle in a Square Well

5.1 The Time-Independent Schrödinger Equation

It is difficult to solve the time-dependent Schrödinger equation explicitly, even in relatively simple cases. (Even for the free Schrödinger equation, we made do in Chap. 4 with solutions that are either approximate or that involve an integral that is not explicitly evaluated.) Usually, then, one analyzes the time-independent Schrödinger equation (the eigenvector equation for $\hat{H}$) and then attempts to infer something about the time-dependent problem from the results. There are a number of problems, including the harmonic oscillator and the hydrogen atom, in which the time-independent Schrödinger equation can be solved explicitly.

In this section, we will consider a simple but instructive example, which can be solved by elementary methods. We consider the time-independent Schrödinger equation in $\mathbb{R}^1$, with a potential of the form

$$V(x) = \begin{cases} -C, & -A \leq x \leq A \\ 0, & |x| > A \end{cases}, \tag{5.1}$$

where A and C are positive constants. The region $-A \leq x \leq A$ is the "square well" for the potential (Fig. 5.1).

Let us think first for a moment about the behavior of a *classical* particle in a square well. If we think of V as the limit of a sequence of potentials that change linearly from -1 to 0 in a small interval around ± 1, we may expect the following behavior for a particle in a square well. If the energy of the particle is negative, then the particle must be in the well. In that

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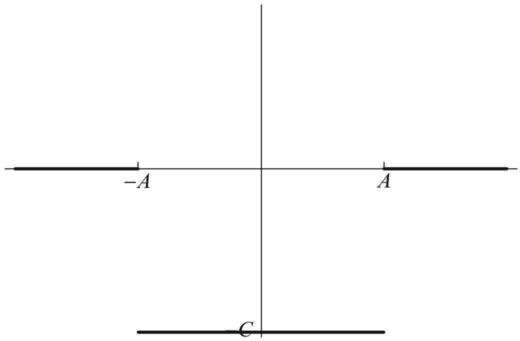

FIGURE 5.1. A square well potential.

case, it will move with constant speed until it hits the edge of the well, at which point it will reflect instantaneously off the wall and move with the same speed in the opposite direction. If the energy of the particle is positive, it will move always in the same direction, with speed equal to one constant when it is not in the well and speed equal to a different constant when it is in the well.

In the quantum case, we will be interested mainly in eigenvectors for the Schrödinger operator with negative eigenvalues ($E < 0$). Of course, on the quantum side of things, energy eigenvectors do not change in time, except for an overall phase factor. Nevertheless, since the classical particle with $E < 0$ spends the same amount of time in each part of the well, we may expect that the quantum particle will have approximately equal *probability* of being found in each part of the well. This expectation will be fulfilled for "highly excited states," such as the one in Fig. 5.7. For the quantum particle, however, there is a small but nonzero probability of finding the particle outside the well, which is impossible classically.

Our goal is to study the time-independent Schrödinger equation, that is, the eigenvalue equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) = E\psi(x), \tag{5.2}$$

where both the eigenvalues E and the associated eigenvectors ψ (or "eigenfunctions," in physics terminology) are as yet unknown. As a second-order linear ordinary differential equation, this equation always has (for any value of E) a two-dimensional solution space. We are, however, looking for solutions that lie in the quantum Hilbert space $L^2(\mathbb{R})$. We will see there are actually only a finitely many E's, all of them with $E < 0$, for which (5.2) has a nonzero solution in $L^2(\mathbb{R})$. In this case, then, the Schrödinger operator $\hat{H}$ has a *discrete spectrum* below zero and a *continuous spectrum* above zero.

5.2 Domain Questions and the Matching Conditions

Before starting to solve (5.2), we must give some heed to the unbounded nature of the Hamiltonian operator. The Schrödinger operator

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(X)$$

on the left-hand side of (5.2) is an *unbounded* operator, meaning that there is no constant C such that $\|\hat{H}\psi\| \leq C\|\psi\|$, where $\|\cdot\|$ is the L^2 norm. On the other hand, we want to define $\hat{H}$ in such a way that it is self-adjoint. But according to Corollary 9.9, a self-adjoint operator that is defined on the whole Hilbert space must be bounded.

We conclude, then, that $\hat{H}$ is not going to be defined on the entire Hilbert space $L^2(\mathbb{R})$, but only on a dense subspace thereof. In practical terms, saying that $\hat{H}$ is not defined on the whole Hilbert space means simply that for many functions ψ in $L^2(\mathbb{R})$, the second derivative $d^2\psi/dx^2$ does not exist, or exists but fails to be in L^2. (In our example, the potential V is bounded, and so $V\psi$ will always be in L^2 provided that ψ is in L^2.)

Since the potential V for a square well is bounded, the domain of the Hamiltonian $\hat{H} = P^2/(2m) + V(X)$ is the same as the domain of the kinetic energy operator $P^2/(2m) = -(\hbar^2/2m)d^2/dx^2$. As we will see in Sect. 9.7, the domain of the kinetic energy operator may be described as the space of L^2 functions ψ for which $d^2\psi/dx^2$, computed in the weak or distributional sense (Appendix A.3.3), again belongs to $L^2(\mathbb{R})$. This condition is equivalent to the statement that there exists some L^2 function ϕ such that ψ is the second integral of ϕ (for some choice of the constants of integration).

Meanwhile, since our potential is piecewise constant, any solution ψ to (5.2) will be smooth except possibly at the transition points $x = \pm A$, and both ψ and ψ' will have left and right limits at A and $-A$. Indeed, on each of the intervals $(-\infty, -A)$, $(-A, A)$, and (A, ∞), any solution to (5.2) will be simply a linear combination of (real or complex) exponentials. For functions of this sort, it is not hard to see when we are in the domain of $\hat{H}$.

Proposition 5.1 *Suppose ψ is smooth on each of the intervals $(-\infty, -A)$, $(-A, A)$, and (A, ∞). Then ψ belongs to the domain of $\hat{H}$ [with potential function given by (5.1)] if and only if the (1) ψ and $d\psi/dx$ are continuous at $x = \pm A$, and (2) $d^2\psi/dx^2$ belongs to $L^2(\mathbb{R})$.*

Proof. Suppose first that ψ satisfies the conditions (1) and (2). Then it is not hard to see (Exercise 1) that the second derivative of ψ in the distribution sense is simply the function $d^2\psi/dx^2$, computed in the ordinary pointwise sense for $x \neq \pm A$. (The second derivative may not exist at $x = \pm A$, but we simply leave $d^2\psi/dx^2$ undefined at these two points, which form a set of measure zero.) Thus, $d^2\psi/dx^2$, computed in the distribution sense, is an element of $L^2(\mathbb{R})$.

On the other hand, if either ψ of ψ' has a discontinuity at $x = A$ or at $x = -A$, then (Exercise 1 again) the distributional derivative will contain either a multiple of a δ-function of a multiple of the derivative of δ-function at one of these points. But neither a δ-function nor the derivative of δ-function is a square-integrable function. ■

Let us think about what the continuity condition on ψ and $d\psi/dx$ means in practical terms. Since V is constant on $(-\infty, -A)$, we can easily solve (5.2) on that interval, obtaining a two-dimensional solution space. Once we choose a solution from this solution space, then the values of ψ and $d\psi/dx$ as x approaches $-A$ from the left will serve as the initial conditions for solving (5.2) on $(-A, A)$. Thus, the requirement of continuity for ψ and $d\psi/dx$ serve as a "matching condition" between the solution on $(-\infty, -A)$ and the solution on $(-A, A)$. We cannot just separately pick any solution to (5.2) on $(-\infty, -A)$ and any solution on $(-A, A)$; at the boundary, the values of ψ and $d\psi/dx$ must match. (This same matching condition appears in elementary treatments of ordinary differential equations with discontinuous coefficients.)

Once we pick a solution on $(-\infty, -A)$ we get a unique solution on $(-A, A)$—and then the values of ψ and $d\psi/dx$ as we approach A from the left will serve as the initial conditions for solving (5.2) on (A, ∞). The conclusion is that once we pick a solution to (5.2) on $(-\infty, -A)$ (from the two-dimensional solution space), we have no additional choices to make; the differential equation along with the matching conditions give a unique way to extend the solution from $(-\infty, -A)$ to the whole real line.

5.3 Finding Square-Integrable Solutions

If $E > 0$, then any solution to (5.2) will be a combination of two complex exponentials in the range $x < -A$; such a function cannot be square-integrable unless it is identically zero. If, however, we take ψ to be identically zero in the region $x < -A$, then our continuity condition requires that ψ and $d\psi/dx$ approach 0 as x approaches $-A$ from the right. Thus, the matching conditions at $-A$ force the solution to be identically zero in $[-A, A]$ as well. Finally, by matching across $x = A$, we get an identically zero solution on $[A, \infty)$. Thus, for $E > 0$, any solution to (5.2) satisfying the continuity conditions in Proposition 5.1 must be identically zero. A similar analysis applies when $E = 0$, where the solutions to (5.2) on $(-\infty, A]$ would be of the form $c_1 + c_2 x$, which is square-integrable only if $c_1 = c_2 = 0$.

The conclusion, then, is that to have a chance to get a solution to (5.2) that is square-integrable and in the domain of $\hat{H}$, we must take $E < 0$. For $E < 0$, the solution to (5.2) on $(-\infty, -A)$ will be a linear combination of the two exponentials $\exp(\alpha x)$ and $\exp(-\alpha x)$, where

$$\alpha = \frac{\sqrt{2m\,|E|}}{\hbar}. \tag{5.3}$$

For ψ to be square-integrable over $(-\infty, -A)$, the coefficient of $\exp(-\alpha x)$ must be zero, since this term grows exponentially as x tends to $-\infty$. Thus, the value of ψ on $(-\infty, -A)$ must be $c\exp(\alpha x)$. Once we choose a value for c, we get a unique solution on $(-A, A)$ by matching ψ and ψ' across $x = -A$. We then get a unique solution on (A, ∞) by matching across $x = A$. The solution on (A, ∞) will be again be a linear combination of $\exp(\alpha x)$ and $\exp(-\alpha x)$. For ψ to be in L^2, we need the coefficient of $\exp(\alpha x)$ on (A, ∞) to be zero. We have no choice, however, about what ψ is on (A, ∞); the coefficient of $\exp(\alpha x)$ either comes out to be zero or it does not.

The conclusion, then, is that for any $E < 0$, there is a unique (up to a constant) solution to (5.2) that is square-integrable on the interval $(-\infty, -A)$. This solution then gives rise to a unique solution on $(-A, A)$ and then to a unique solution on (A, ∞), up to a constant. Unless we are lucky, the solution on (A, ∞) will grow exponentially and thus fail to be in L^2. Therefore, in most cases there will be no nonzero solution to (5.2) that satisfies the continuity condition and is square-integrable over the whole real line. The hope is that for *certain special values of* E, we will be able to find a solution that decays exponentially *both* on $(-\infty, -A)$ and on (A, ∞), in which case the solution will belong to $L^2(\mathbb{R})$.

It can be shown (Exercise 6) that there are no nonzero square-integrable solutions with $E \leq -C$. Therefore, any square-integrable solutions to (5.2) that may exist must come from the range $-C < E < 0$. To analyze this range, let us rewrite the time-independent Schrödinger equation by dividing through by $-\hbar^2/(2m)$, yielding the equation

$$\frac{d^2\psi}{dx^2} = \begin{cases} \varepsilon\psi & |x| > A \\ -(c-\varepsilon)\psi & |x| < A \end{cases}. \tag{5.4}$$

where

$$\begin{aligned} \varepsilon &= -\frac{2mE}{\hbar^2} \\ c &= \frac{2mC}{\hbar^2}. \end{aligned} \tag{5.5}$$

Note that although E is assumed to be negative, we have normalized ε to be positive; the condition $-C < E < 0$ corresponds to $0 < \varepsilon < c$.

Because our potential function V is even, it is easy to see that for any solution ψ to (5.4), the even and odd parts of ψ are also solutions. We can, therefore, analyze even solutions and odd solutions separately. We begin with the even case. For $x < -A$, every solution to (5.4) that is square-integrable over $(-\infty, A)$ is of the form

$$\psi(x) = ae^{\sqrt{\varepsilon}x}, \quad x \leq -A. \tag{5.6}$$

Since we assume that ψ is even, we then have

$$\psi(x) = ae^{-\sqrt{\varepsilon}x}, \quad x \geq A. \tag{5.7}$$

Meanwhile, for $-A < x < A$, every even solution is of the form

$$\psi(x) = b\cos\left(\sqrt{c-\varepsilon}x\right). \tag{5.8}$$

Proposition 5.2 *Let ψ be the function defined in (5.6)–(5.8). Then there exist nonzero constants a and b so that ψ belongs to the domain of $\hat{H}$ if and only if the following matching condition holds:*

$$\sqrt{\varepsilon} = \sqrt{c-\varepsilon}\tan\left(\sqrt{c-\varepsilon}A\right). \tag{5.9}$$

Proof. Clearly both ψ and $d^2\psi/dx^2$ belong to $L^2(\mathbb{R})$. Thus, in light of Proposition 5.1, we need only ensure that $\psi(x)$ and $\psi'(x)$ are continuous at $x = \pm A$. Since the exponential functions are never zero, we may always ensure that ψ itself is continuous by taking any value we like for b and then choosing a appropriately Once ψ has been made to be continuous, ψ' will be continuous provided that $\psi'(x)/\psi(x)$ has the same value as we approach $\pm A$ from inside the well or from the outside. To obtain the condition (5.9), we compute ψ'/ψ from (5.6) and then from (5.8), evaluate both quantities at $x = -A$, and then equate the two values of ψ'/ψ. Because we have made our solution an even function, we get the same matching condition at $x = A$ as at $x = -A$.

Now, in deriving (5.9), we implicitly assumed that ψ is nonzero at $x = \pm A$. We do not, however, get any nonzero solutions in which $\psi(\pm A) = 0$. After all, at points where the cosine function in (5.8) is zero, its derivative is nonzero. But no choice of the constant in front of the exponentials (5.6) and (5.7) will produce a function that is zero but has a derivative that is nonzero. ■

Proposition 5.3 *For all positive values of c and A, there exists at least one $\varepsilon \in (0, c)$ such that (5.9) holds.*

Proof. Case 1: $\sqrt{c}A < \pi/2$. In this case, as ε varies between 0 and c, the left-hand side of (5.9) will vary between 0 and some positive number, whereas the right-hand side of (5.9) will vary between some positive number and 0. By the intermediate value theorem, there must exist $\varepsilon \in (0, c)$ for which (5.9) holds. See Fig. 5.2.

Case 2: $\sqrt{c}A \geq \pi/2$. In this case, there is $\varepsilon_0 \in [0, c]$ for which $\sqrt{c - \varepsilon_0}A = \pi/2$. As ε decreases from c to ε_0, the right-hand side of (5.9) will vary from 0 to $+\infty$. Thus, for ε slightly larger than ε_0, the right-hand side of (5.9) will be larger than the left-hand side. By the intermediate value theorem, there must exist $\varepsilon \in (\varepsilon_0, c)$ for which (5.9) holds. See Fig. 5.3 for a case $\sqrt{c}A$ slightly larger than $\pi/2$ and Fig. 5.4 for a case with $\sqrt{c}A$ much larger than $\pi/2$. ∎

Note that if $\sqrt{c}A$ is much larger than $\pi/2$, then there will be multiple solutions of (5.9), as can be seen in Fig. 5.4.

We have found, then, at least one solution ψ to (5.4) that satisfies the matching condition and for which both ψ and ψ'' decay exponentially at infinity. Since this ψ belongs to the domain of $\hat{H}$, we have established the following result.

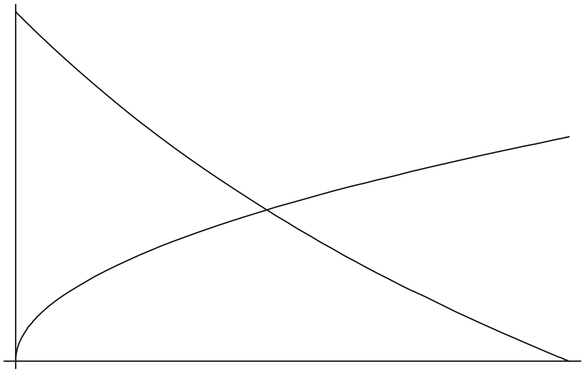

FIGURE 5.2. Solving the matching condition, Case 1.

Proposition 5.4 *For any positive values of A and C, there exists at least one value of E in the range $-C < E < 0$ for which (5.2) has a nonzero solution in the domain of $\hat{H}$, given by the formula*

$$\psi(x) = \begin{cases} \cos\left(\sqrt{c - \varepsilon}x\right) & -A \leq x \leq A \\ \cos\left(\sqrt{c - \varepsilon}A\right)\exp[-\sqrt{\varepsilon}(|x| - A)] & |x| \geq A \end{cases},$$

where c and ε are defined in (5.5) and where ε satisfies (5.9).

In Proposition 5.4, we have *not* normalized ψ to be a unit vector in $L^2(\mathbb{R})$, but rather have normalized ψ to equal 1 at the origin. In Figs. 5.5–5.7, we plot our eigenfunction in several different cases. In Fig. 5.5, we have a "shallow" well, with $\sqrt{c}A = 1$. In that case, we obtain only one even eigenvector, which is the *ground state* of the system (i.e., the eigenvector with the smallest eigenvalue). Next, we consider a "deep" well, with $\sqrt{c}A = 30$. For this well, the ground state is shown in Fig. 5.5 and an "excited state"

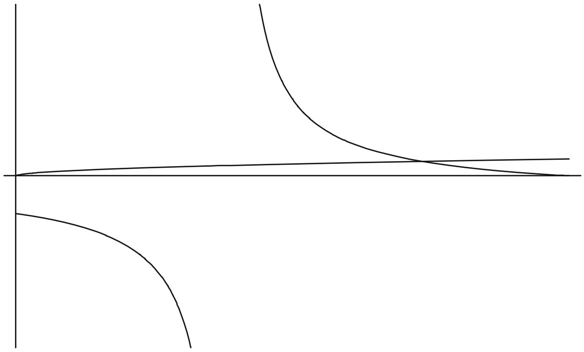

FIGURE 5.3. Solving the matching condition, Case 2a.

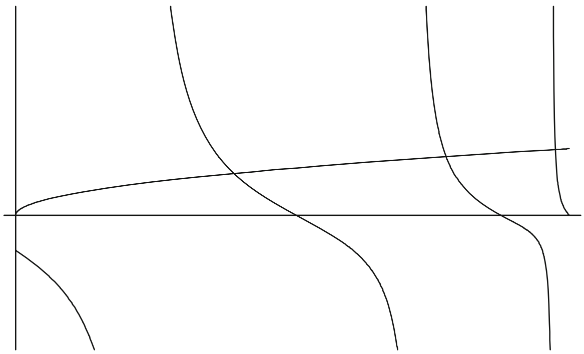

FIGURE 5.4. Solving the matching conditions, Case 2b.

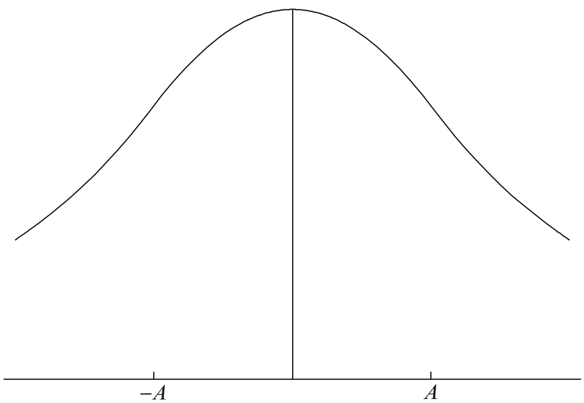

FIGURE 5.5. Ground state for a shallow potential well.

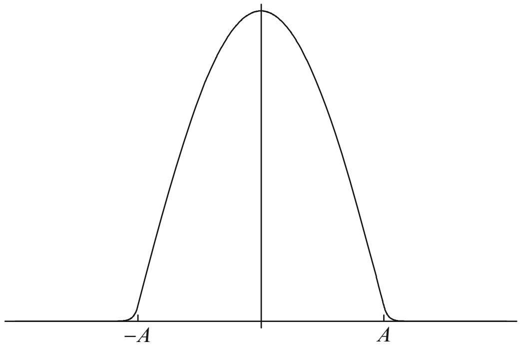

FIGURE 5.6. Ground state for a deep potential well.

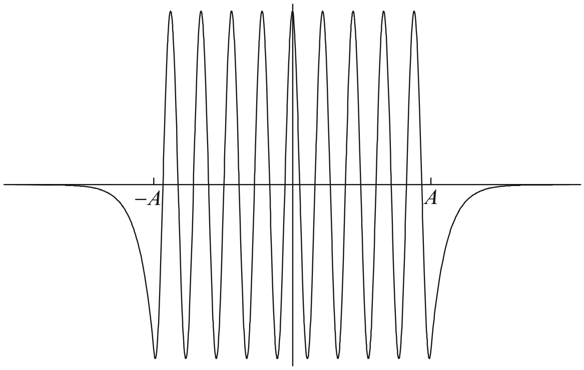

FIGURE 5.7. Excited state for a deep potential well.

(i.e., an eigenvector with an eigenvalue that is not the smallest) is shown in Fig. 5.7.

Note that in the shallow well, the ground state extends quite a bit beyond the interval $[-A, A]$, whereas in the deep well, the ground state goes to zero very quickly as soon as we move outside the well. On the other hand, the excited state in Fig. 5.7 extends comparatively far outside the well.

It is straightforward to adapt the preceding analysis to the odd case. The matching condition (5.9) is replaced by

$$\sqrt{\varepsilon} = -\sqrt{c-\varepsilon}\cot\left(\sqrt{c-\varepsilon}A\right) \tag{5.10}$$

(Exercise 2) and the formula for the eigenvectors is now

$$\psi(x) = \begin{cases} \sin\left(\sqrt{c-\varepsilon}x\right) & -A \leq x \leq A \\ \pm\sin\left(\sqrt{c-\varepsilon}A\right)\exp[-\sqrt{\varepsilon}(|x|-A)] & |x| \geq A \end{cases},$$

where we take the $+$ sign for $x > A$ and the $-$ sign for $x < -A$.

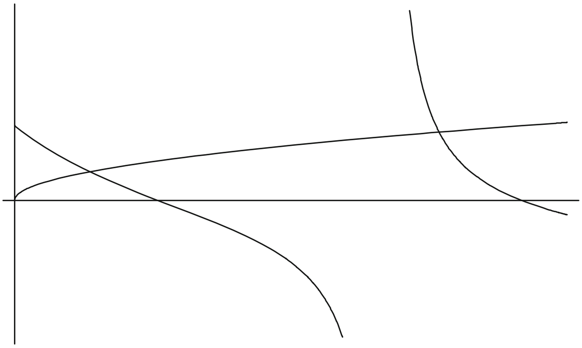

FIGURE 5.8. Matching condition for odd solutions.

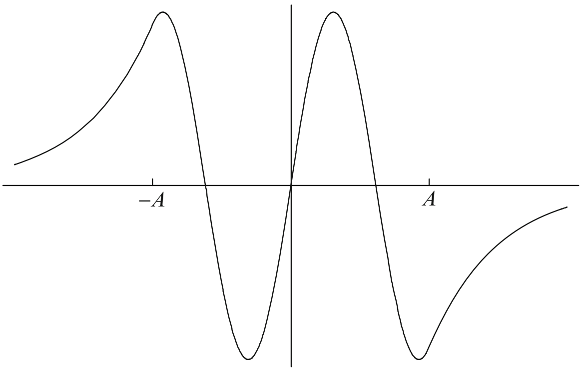

FIGURE 5.9. An odd solution.

If $\sqrt{c}A < \pi/2$, then the matching condition (5.10) will have no solutions, since the right-hand side of (5.10) will be negative for all $\varepsilon \in (0, c)$. For large values of $\sqrt{c}A$, there will be several solutions to (5.10). A typical matching scenario and an associated eigenfunction are plotted in Figs. 5.8 and 5.9.

5.4 Tunneling and the Classically Forbidden Region

Let us now briefly compare the classical situation to the quantum one. Classically, if a particle has energy E, then since the kinetic energy $p^2/(2m)$ is always non-negative, the particle simply cannot be located at a point x with $V(x) > E$. Thus, the region $V(x) \leq E$ may be called the "classically allowed" region and the region $V(x) > E$ the "classically forbidden" region. In the case of a square well potential (5.1), if $-C < E < 0$, then the "well" itself (i.e., the region with $-A \leq x \leq A$) is the classically allowed region and the outside of the well (i.e., the region with $|x| > A$) is the classically forbidden region.

Quantum mechanically, if $\hat{H}\psi = E\psi$, then the particle has a definite value for the energy, namely E. We see, however, that such a particle has a nonzero probability of being located in the classically forbidden region. Note that although the wave function is not zero in the classically forbidden region, it does decay exponentially with the distance from the classically allowed region. That is to say, the quantum particle can penetrate some distance into the classically forbidden region. Note, however, that if E is much less than zero—i.e., ε is large—then a state with $\hat{H}\psi = E\psi$ will decay very rapidly outside the well (like $\exp[-\sqrt{\varepsilon}(|x| - A)]$).

More generally, we can think about the time-dependent Schrödinger equation for a particle with energy *approximately* equal to E. If we require that the energy be *exactly* equal to E, then there is no interesting time-dependence, since the solution to the time-dependent Schrödinger equation is simply a constant time ψ_0. We can, however, think of a particle where the uncertainty in the energy is nonzero but small. Suppose such a particle is traveling through a region with $V < E$ and then approaches a region with $V > E$ (a "potential barrier"). Classically, the particle would just reflect off of this barrier and go back in the other direction. Quantum mechanically, though, it is possible for the particle to "tunnel" through the potential barrier and come out the other side. That is to say, at some later time, there will be some non-negligible portion of the wave function on the far side of the barrier.

5.5 Discrete and Continuous Spectrum

Our analysis of the eigenvector equation (5.2) for $-C < E < 0$ shows that there are only finitely many values of E in this range for which we get square-integrable solutions. It is not hard to analyze the case $E \leq -C$ with the result that all nonzero solutions grow exponentially in at least one direction (Exercise 6). Meanwhile, for $E > 0$, any solution to (5.2) on $(-\infty, -A)$ has sinusoidal behavior and is not square-integrable unless it is identically zero, in which case (by our matching condition) the solution must be zero everywhere.

The upshot is that we obtain only finitely many square-integrable solutions to (5.2), up to multiplying each solution by a constant. Clearly, then, the "true" eigenvectors for $\hat{H}$ [i.e., the ones that actually belong to the Hilbert space $L^2(\mathbb{R})$] cannot form an orthonormal basis for $L^2(\mathbb{R})$. Nevertheless, the spectral theorem (Chap. 7) provides something like a orthonormal-basis decomposition of elements of $L^2(\mathbb{R})$ in terms of the solutions to (5.2). A general element ψ of $L^2(\mathbb{R})$ will be a sum of two terms. The first term is a linear combination of the true (L^2) eigenvectors for

$\hat{H}$, which have $E < 0$. The second term is a continuous superposition (i.e., an integral) of the non–square-integrable "generalized eigenvectors" with $E > 0$.

In Chap. 9, we will introduce the notion of the *spectrum* of a (possibly unbounded) self-adjoint operator A. We will see that a number λ belongs to the spectrum of A if for all $\varepsilon > 0$ there exists a unit vector ψ in the domain of A for which $\|A\psi - \lambda\psi\| < \varepsilon$. In the case of the Hamiltonian operator $\hat{H}$ with a square well potential, it is not hard to show that every real number E with $E \geq 0$ belongs to the spectrum of $\hat{H}$ (Exercise 4.).

It can be shown that if a number $E < 0$ is not an eigenvalue (i.e., if there are no nonzero L^2 solutions to $\hat{H}\psi = E\psi$), then E is not an element of the spectrum of $\hat{H}$. This result is hinted at by Exercise 5. Thus, the spectrum of $\hat{H}$ consists of a finite number of points in $(-C, 0)$ (at least one), together with the whole half line $[0, \infty)$.

5.6 Exercises

1. (a) Suppose ψ is a smooth function on each of the intervals $(-\infty, -A)$, $(-A, A)$, and (A, ∞) and that both ψ and ψ' are continuous at $x = A$ and at $x = -A$. Show that for any smooth function χ with compact support, we have

$$\int_{-\infty}^{\infty} \chi''(x)\psi(x)\ dx = \int_{-\infty}^{\infty} \chi(x)\psi''(x)\ dx, \tag{5.11}$$

where we leave $\psi''(x)$ undefined at $x = \pm A$ if the second derivative does not exist at those points. (In light of Definition A.28, (5.11) means that the second derivative of ψ, in the distribution sense, is simply the function ψ''.)

Hint: Choose some interval $[-R, R]$ with $R > A$ containing the support of χ. Now use integration by parts separately on each of the intervals $[-R, -A]$, $[-A, A]$, and $[A, R]$, paying careful attention to the boundary terms.

(b) Suppose now that ψ is a smooth function on each of the intervals $(-\infty, -A)$, $(-A, A)$, and (A, ∞), and that both ψ and ψ' have left and right limits at $x = \pm A$, but that, say, ψ' has a discontinuity at $x = -A$. Show that (5.11) has to be modified by adding a nonzero multiple of $\chi(-A)$ to the right-hand side.

2. Verify the matching condition (5.10) for odd solutions of the time-independent Schrödinger equation.

3. Let ω be a nonzero real number and consider a function of the form

$$\psi(x) = a\cos(\omega x) + b\sin(\omega x),$$

for real numbers a and b. If a and b are not both zero, show that for any $A \in \mathbb{R}$, we have

$$\lim_{B \to +\infty} \int_A^B \psi(x)^2 \, dx = +\infty.$$

4. Let f be a C^∞ function on the interval $(0, 1)$ with the property that $f(x) = 1$ for $0 < x < 1/3$ and $f(x) = 0$ for $2/3 < x < 1$. Then define a family of "cutoff" functions χ_n on $\mathbb{R}$ by the formula

$$\chi_n(x) = \begin{cases} 0 & |x| \geq n+1 \\ 1 & |x| \leq n \\ f(-x-n) & -(n+1) < x < -n \\ f(x-n) & n < x < n+1 \end{cases}.$$

Given any $E > 0$, let ψ be a nonzero solution to (5.2) for which $\psi(x)$ and $\psi'(x)$ are continuous at $x = \pm A$. Let $\psi_n = \psi\chi_n$. Show that ψ_n belongs to the domain of $\hat{H}$ and that

$$\lim_{n \to \infty} \frac{\left\| \hat{H}\psi_n - E\psi_n \right\|}{\|\psi_n\|} = 0.$$

Note: As we will see in Chap. 9, this implies that every real number E with $E > 0$ belongs to the *spectrum* of the operator $\hat{H}$.

Hint: In estimating $\|\psi_n\|$, it may be helpful to apply Exercise 3 to the real and imaginary parts of ψ outside the well.

5. Suppose $E < 0$ and suppose that there exists no nonzero square-integrable solutions to (5.2) for which ψ and ψ' are continuous. Let ψ be a nonzero solution of (5.2) for which $\psi(x)$ and $\psi'(x)$ are continuous at $x = \pm A$ and let ψ_n be as in Exercise 4. Show that

$$\frac{\left\| \hat{H}\psi_n - E\psi_n \right\|}{\|\psi_n\|}$$

does not tend to zero as n tends to infinity.

6. (a) Show that for $E < -C$, there are no nonzero square-integrable solutions to (5.2) for which ψ and ψ' are continuous.

   (b) Obtain the result of Part (a) when $E = -C$.

   Hint: Analyze the even and odd cases separately.

7. Let the *ground state* for a particle in a square well denote the eigenvector with the lowest (most negative) eigenvalue, which corresponds to the largest value for ε.

(a) Show that the ground state is always an even function. That is to say, show that the largest value of ε satisfying (5.9) is always larger than any solution to (5.10).

(b) Show that the ground state is a nowhere-zero function.