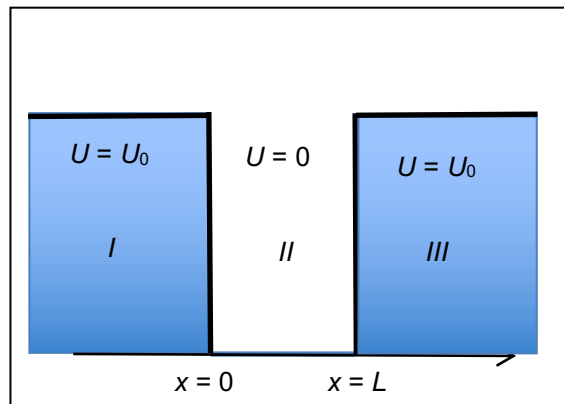


## Schrödinger, 2

### The finite square well

The infinite square well potential energy rigorously restricts the associated wavefunction to an exact region of space: it is *infinitely “hard.”* Potential energies encountered in more realistic physical scenarios are “softer” in that they permit wavefunctions to spread throughout less well-defined regions. An important toy example of the latter is the **finite square well**. In this problem, the potential energy function is

$U(x) = 0$ , if  $0 < x < L$ , and  $U_0$  otherwise. See the figure to the right. As previously, we try to find energy eigenstates by separating the space and time parts of the Schrödinger



Equation:  $\Psi(x,t) = X(x)T(t)$  with  $T(t) \propto \exp(-iEt/\hbar)$  and  $\frac{d^2X}{dx^2} = -\frac{2m}{\hbar^2}[E - U(x)]X$ . There are two cases of interest, namely, when the particle’s energy is less than or greater than  $U_0$ .

Let’s examine **the  $E < U_0$  case** first. The quantity  $E - U(x)$  is the classical kinetic energy of the particle. In region II the kinetic energy is just  $E$ , while in regions I and III the kinetic energy,  $E - U_0$ , should be negative. That is, if the particle were a classical particle it would be forbidden to be in I and III. But quantum particles are described by wavefunctions that slosh about. For the infinite square well the particle was forbidden in I and III because the potential energy was infinite there, but no such exclusion can be invoked for the finite well. In

particular,  $\frac{d^2X}{dx^2} = K^2X$ , in I and III, where  $K = \sqrt{\frac{2m(U_0 - E)}{\hbar^2}}$ . This equation has solutions of the form  $X \propto \exp(\pm Kx)$ , where these are *real* exponentials (i.e., they have no wiggles). In II,

$\frac{d^2X}{dx^2} = -k^2X$ , where  $k = \sqrt{\frac{2mE}{\hbar^2}}$ . As long as  $E > 0$ , solutions in II are of the form

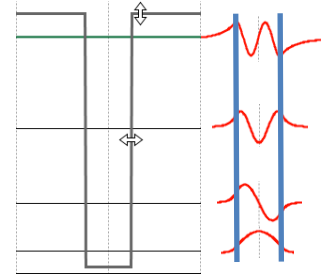
$\sin(kx)$ ,  $\cos(kx)$ ,  $\exp(\pm ikx)$  (i.e., they *do* have wiggles). (If  $E \leq 0$ , the problem has no solutions.) So, the problem becomes how to manufacture a smoothly continuous wavefunction that doesn’t wiggle in I and III but does in II, because  $K$  and  $k$  suddenly switch at the well boundaries. **(The wavefunction has to be smoothly continuous because otherwise its derivatives will blow up where it isn’t—leading to infinite kinetic energies.)**

Not all of the possibilities listed above are allowed. The integral of  $|\Psi|^2$  over all  $x$  values has to be 1, but it would blow up as  $x \rightarrow -\infty$  in region I if  $X \propto \exp(-Kx)$ ; thus that possibility has to be discarded as unphysical. Similarly,  $X \propto \exp(Kx)$  has to be discarded in region III. To smoothly match solutions in I and II at  $x = 0$  and in II and III at  $x = L$  requires finding values of  $K$  and  $k$  (i.e., particle energies) for which

$$X_I(0) = X_{II}(0), \quad X_{II}(L) = X_{III}(L), \quad X'_I(0) = X'_{II}(0), \quad X'_{II}(L) = X'_{III}(L),$$

where the primes mean “derivative with respect to  $x$ .” It is not very instructive to do the algebra associated with this string of equations but, in the end,  $K$  and  $k$  have a (nasty, transcendental) relation that can be only solved numerically for the energy  $E$  that makes this relation true. Only

certain energies are allowed. The figure to the right shows the example of an electron in a well with  $L = 0.5 \text{ nm}$  and  $U_0 = 17 \text{ eV}$ . For this case, there are only four allowed states with energies 1.07 eV, 4.22 eV, 9.26 eV, and 15.47 eV. (For comparison, the first four energy eigenvalues in an infinite square well with the same  $L$  are: 1.50 eV, 6.00 eV, 13.50 eV, and 24.00 eV.) The spatial wavefunctions corresponding to these energies are shown to the right of the well. Notice that as energy increases the tails of the wavefunctions leak out more and more into the classically forbidden regions. Because of this leakage, the finite well wavefunctions don't wiggle as abruptly as the corresponding infinite well wavefunctions; the magnitudes of their momenta (proportional to their derivatives) are not as large. The ground state wavefunction is most like that for the infinite well and its energy is closest to the ground state infinite well energy; the fourth states, in the example, are least like one another and so are their energies. As the finite well is made shorter or as  $U_0$  is made less, fewer bound states are allowed. Nonetheless, it is a fact that **a finite square well always contains at least one bound state**.



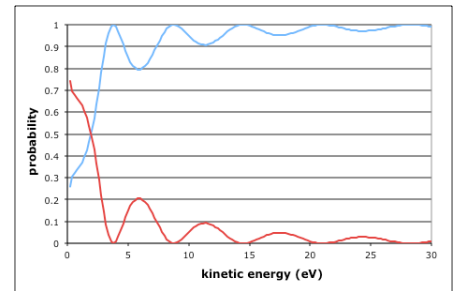
Now let's examine the  $E > U_0$  case. In this case, in regions I and III  $\frac{d^2 X}{dx^2} = -K^2 X$ ,

where  $K = \sqrt{\frac{2m(E - U_0)}{\hbar^2}}$ , and in region II (as before)  $\frac{d^2 X}{dx^2} = -k^2 X$ , where  $k = \sqrt{\frac{2mE}{\hbar^2}}$ . In this

case, there are wiggling wavefunctions in all three regions that have to be smoothly matched at the well boundaries. Suppose that in region I there is a plane wave traveling to the right ("incident" on the well) of the form  $\Psi = \exp[i(Kx - \omega t)]$ . *Plane waves can't be normalized* because their square amplitudes are  $\geq 0$  everywhere, but all other wavefunctions in this problem can have amplitudes relative to an arbitrarily assigned amplitude of the "incident" plane wave, which might as well be chosen to be 1. At  $x = 0$  and  $x = L$  the wavelength abruptly changes. **Whenever a traveling wave (irrespective of whether it is electromagnetic, elastic, or probabilistic) undergoes a wavelength change the requirement of smooth matching can only be met if there is a reflected wave.** This presents a quantum mechanical surprise: a *particle traveling left to right speeds up on entering the well at  $x = 0$ , yet, in general, has some probability of being reflected back to the left*, i.e., some probability of being "back scattered." If you fire an electron directly at a proton, there's a probability it will come back at you! That would never happen to a classical particle, which would just keep going through the well region and appear in region III with 100% probability.

When the particle speeds up at  $x = 0$  (remember kinetic energy =  $E - U$ ), its de Broglie wavelength decreases. In terms of wavelength, this is like light entering a piece of glass with index of refraction  $> 1$ ; the wavelength decreases (though for light, the effective speed *decreases*). At such a face the reflected light undergoes a  $180^\circ$  phase change relative to the incident light. At  $x = L$  the wavelength abruptly increases (as the particle slows down). This is like light leaving the glass (except the effective speed increases for light); the reflected light at this face does not change phase. The reflected wave in region I is the sum of a wave immediately reflecting from  $x = 0$ , plus waves propagating to the left after traveling integral multiples of  $2L$  (the total path length for a wave entering the well, reflecting from  $x = L$ , then leaving the well at  $x = 0$ ). If  $2L$  is an integral number of wavelengths of the particle in the well, then this sum adds up to zero. This is the condition for perfect transmission—no reflected wave in region I. The figure below shows how the transmission (upper, blue curve) and reflection (lower, red curve) probabilities vary with incident kinetic energy for an electron incident on a well

with  $U_0 = 10$  eV and  $L = 0.5$  nm. (The figure is generated by numerically solving the smooth matching problem for waves at  $x = 0$  and  $L$ .) When  $2L$  equals an integral number of the electron's wavelength in the well, there is 100% transmission and no reflection. Note that as the electron's incident kinetic energy becomes larger and larger, the electron tends to pass through the well region more and more, just like a classical particle.



**Example:** What is the lowest incident kinetic energy for the well in the figure for 100% transmission of the electron?

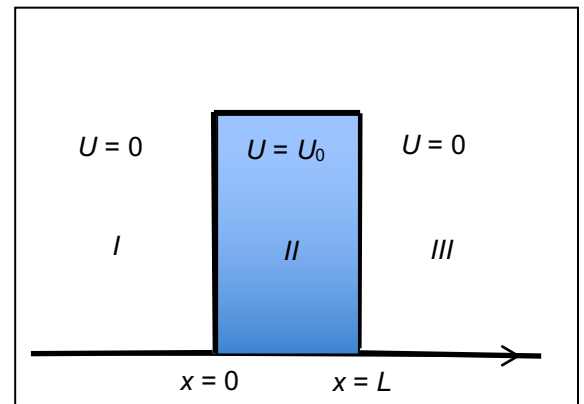
**Solution:** For 100% transmission,  $\lambda = 2L/n$ . This is just the wavelength criterion for eigenstates in an infinite square well of length  $L$ . Thus, the energies associated with the electron motion that meet the wavelength criterion are  $E_n = (n\pi\hbar c)^2 / 2mc^2 L^2 = 1.50n^2$  eV (for this well length). In order for the particle's energy to be greater than 10 eV (the well depth) it must be that  $n \geq \sqrt{10/1.5} = 2.58$ . The first integer for which this condition is satisfied is 3. Thus, the lowest total energy the particle can have is 13.50 eV and its incident and final kinetic energy must be  $13.50$  eV  $-$   $10$  eV =  $3.50$  eV.

The importance of scattering and transmission experiments is that by varying the energy of one particle incident on a second the details of a model potential energy associated with the interaction of the two can be fully extracted.

### Tunneling

A closely related problem to scattering from a well is scattering from and tunneling through a repulsive potential energy barrier (as to the right). When  $E > U_0$  the situation is similar to scattering from an attractive well (i.e., reflection as well as transmission). When  $E < U_0$  the particle's kinetic energy within the barrier region is negative; this is a classically forbidden region. A classical particle incident from the left in region *I* would reflect back into *I* with 100% probability. A quantum wavefunction, however, can leak into the forbidden region, *II*, and also show up in region *III*. That means there is some probability that the particle can get through the repulsive barrier. This is called "tunneling."

**The particle in region III has the same energy as in region I, but the amplitude of the wavefunction is reduced.** Solutions to the Schrödinger equation are wiggling functions in *I* and *III*, but real (growing and dying) exponentials in *II*. Of course, as before, wavefunction solutions require smooth matching at the barrier boundaries, but an order of magnitude estimate for the tunneling probability ( $T$ ) is given by the square of the dying exponential in the barrier region:  $T \sim \exp(-2KL)$ , where  $K = \sqrt{2m(U_0 - E)/\hbar^2}$ .



Example: Suppose  $U_0 - E = 1 \text{ eV}$ . If the incident particle is an electron, then  $K = 5.13 \text{ nm}^{-1}$ . A plot of tunneling probability versus barrier length for this case is shown to the right. Note that tunneling probability drops very rapidly as  $L$  increases. This behavior is the basis for the scanning tunneling microscope (STM), in which electrons tunnel between a sharp wire tip and a solid surface. By carefully adjusting the tip-to-surface distance to keep the tunneling current constant as the tip is rastered over the surface it is possible to map out the height of atoms on the surface. A typical STM image (here, of silicon atoms on a solid surface) is shown to the below. From <http://www.exo.net/~pauld/workshops/Atoms.html>.

