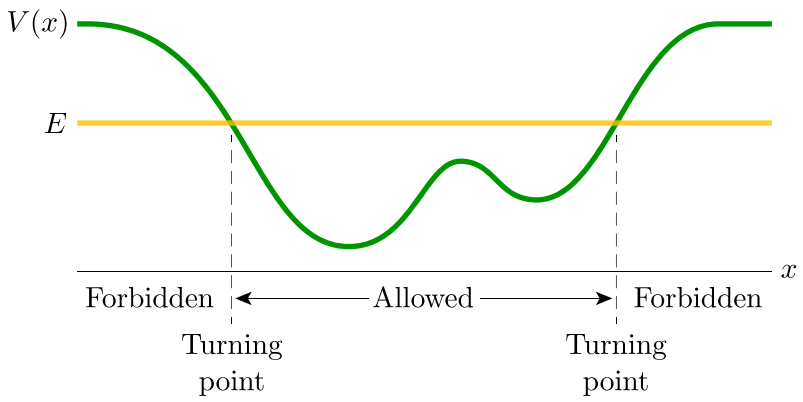
6. Qualitative Solutions of the TISE

Our goal for the next few lessons is to solve the time-independent Schrödinger equation (TISE) for a variety of one-dimensional potential functions $V(x)$. That is, we want to find the energy levels and corresponding energy eigenfunctions for a quantum particle subject to a variety of types of forces. Some of these examples will have important real-world applications, for example, to molecular vibrations or to electrons in semiconductors.

We've already worked out the solutions for the infinite square well, so a logical next step would be to pick a slightly more complicated $V(x)$—perhaps a square well with a finite depth, or the smooth potential of a simple harmonic oscillator—and work out its solutions. But before we do that, I'd like to step back and ask what the solutions to the TISE look like *in general*. We can actually gain quite a bit of understanding by just looking at the TISE, thinking about it qualitatively, and drawing a bunch of pictures.

So consider a generic potential energy function $V(x)$, which might look like this:



I've also drawn a horizontal line, at an arbitrary level, to indicate the total energy E of a hypothetical particle that's subject to this potential.

Now if this were a *classical* particle, we could immediately determine the qualitative features of the motion from this diagram. We would first note that the particle's kinetic energy,

$$K = E - V(x), \tag{1}$$

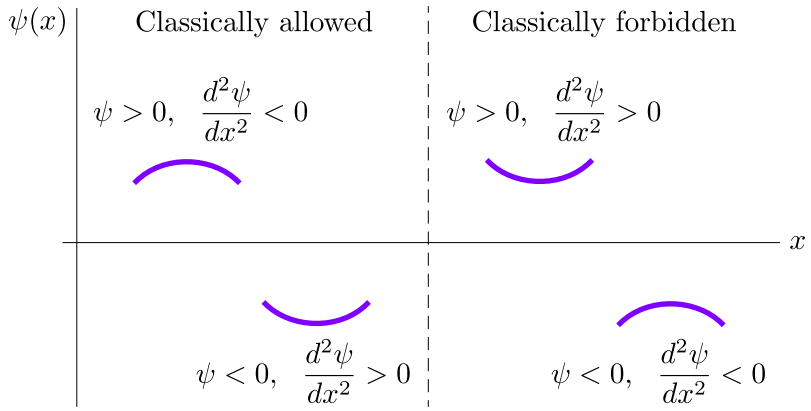
cannot be negative, so any x where E is less than $V(x)$ is *classically forbidden*: the particle simply cannot be there if its total energy is only E. The locations where E is greater than $V(x)$ are similarly called *classically allowed*. Within a classically allowed region, the particle will be moving faster where $V(x)$ is smaller (large K) and slower where $V(x)$ is larger (small K). The boundaries between the classically allowed and forbidden regions are called *classical turning points*: a particle at one

of these locations must have just come to rest ($K = 0$), after moving in from the allowed region and before moving back into the allowed region. Remember that the *force* on the particle is minus the slope of the potential energy: $F_x = -dV/dx$.

The distinction between allowed and forbidden regions is also critical in quantum mechanics, although we'll see that the word "forbidden" is somewhat of a misnomer. We're interested in wavefunctions with definite energy, so let's look at the TISE, which these functions must obey:

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

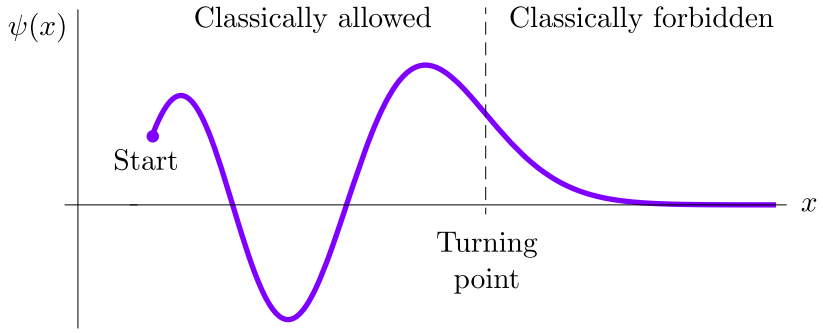
First note that there are no i's in this equation, so we can always find solutions that are purely real; I'll take ψ to be real for the rest of this lesson. Now focus on the factor $(E - V(x))$ in the TISE. This factor is positive in an allowed region but negative in a forbidden region, and this sign change dramatically affects the shape of the solution $\psi(x)$. In an allowed region, ψ and its second derivative have *opposite* signs, while in a forbidden region, ψ and its second derivative have the *same* sign. The second derivative indicates the *curvature* of the graph of $\psi(x)$: concave-up or concave-down. Thus, $\psi(x)$ curves *toward* the x axis in an allowed region and *away from* the x axis in a forbidden region:



This picture shows the four different possibilities for the signs of ψ and $d^2\psi/dx^2$. Not shown are the borderline cases where $d^2\psi/dx^2 = 0$ (an "inflection point"), either at a classical turning point ($E = V(x)$) or where ψ crosses the x axis.

Now let's imagine drawing a sketch of $\psi(x)$, for some given energy. There's no obvious way to get started, so for now I'll just arbitrarily say that we can start with some positive ψ value and some positive slope ($d\psi/dx$), at some particular x value that lies in a classically allowed region (see the figure on the next page). Then, by the TISE, the graph must be concave-down at this point, so as we move the pencil to the right we should curve downward through a local maximum and then continue downward until the graph crosses the x axis, at which point its curvature will have

decreased to zero. Continuing to the right, the graph goes below the x axis but now begins curving upwards, so it then reaches a local minimum and heads back up, crossing the x axis again and finishing a complete "cycle."



If the potential energy $V(x)$ were *constant* throughout this range of x values, then this oscillation cycle would be a perfect sine wave (as you can easily show from the TISE). In general $V(x)$ will not be constant, so the "wavelength" and "amplitude" of $\psi(x)$ will vary from place to place. You can use the TISE to figure out exactly how they vary,[1] but it's easier to go back to more basic principles. The de Broglie relation tells us that wavelength increases as the kinetic energy ($p^2/2m$) decreases, or as the potential energy increases. That is, the "waves" will be more spread-out horizontally in locations where $V(x)$ is larger. And the amplitude (that is, the vertical size) of the oscillations will be larger in these locations as well, in agreement with our classical intuition that a particle is more likely to be found in places where it's moving more slowly. Looking at the picture above, you can see that I drew oscillations that grow larger (both horizontally and vertically) from left to right, so I've assumed that $V(x)$ increases from left to right in the classically allowed region.

Eventually, however, as we move along in x we'll usually come to a classical turning point. There the curvature of the graph goes to zero and on the other side the curvature changes sign. In my picture above, this happens where ψ is positive, so the curvature changes from concave-down, in the classically allowed region on the left, to concave-up, in the classically forbidden region on the right. Often (though not always) the forbidden region extends indefinitely to the right, and in that case the *only* consistent behavior for $\psi(x)$ is to die out asymptotically to zero. (The TISE would also allow ψ to grow to infinity, but such a wavefunction wouldn't be normalizable.) In the special case where $V(x)$ is *constant* throughout some or all of the classically forbidden region, you can easily show that $\psi(x)$ must be an exponential function of the form $e^{-\kappa x}$, where κ depends on the difference between V and E. More specifically, a large value of $V - E$ implies a large κ, which makes the

[1] A. P. French and E. F. Taylor, "Qualitative Plots of Bound State Wave Functions," American Journal of Physics **39**(8), 961–962 (1971).

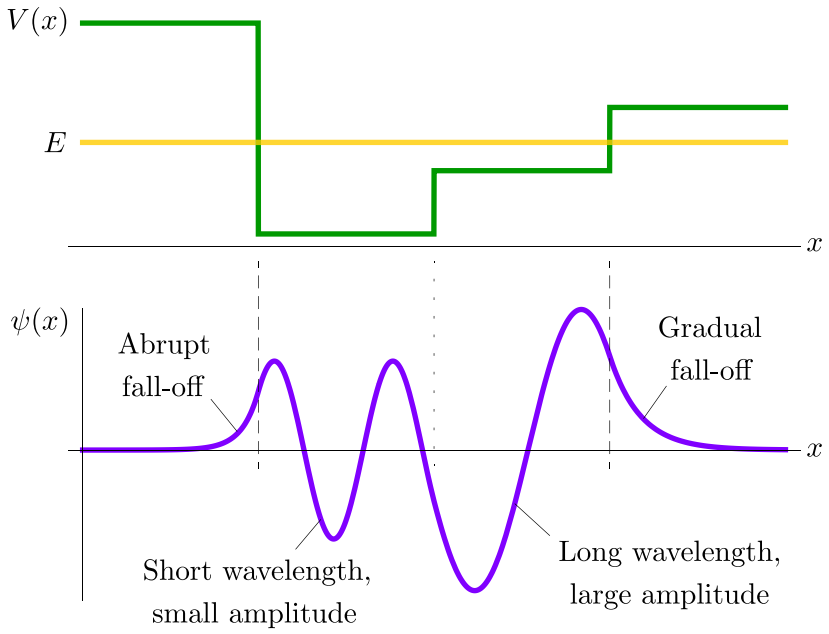
wavefunction die out more abruptly. And if there is a classically forbidden region on the left, the wavefunction will die out asymptotically over there as well, taking the form $e^{+\kappa x}$ in the special case where $V(x)$ is constant.

While it is intuitively pleasing that wavefunctions tend to die out exponentially in classically forbidden regions, you may be wondering how it's possible for the wavefunction in these regions to be nonzero at all. How can there be a nonzero probability of finding a particle in a location where its potential energy is greater than its total energy? This behavior is one of the many wonders of quantum mechanics, and is a consequence of the TISE. And there's no actual paradox, because the process of measuring a particle's position can change its energy, or, more precisely, put the particle into a state for which its energy isn't even well defined.

In summary, the solutions to the TISE have the following properties:

- In a classically allowed region, the solutions oscillate. Both the amplitude and the wavelength of the oscillations will be smaller where $E - V(x)$ is large.
- In a classically forbidden region, the solutions have exponential-like behavior, dying out as the distance from a classically allowed region increases. The wavefunction dies out more abruptly where $V(x) - E$ is large.

Here is an example to illustrate all of these properties, using a piecewise-constant potential function, with four different levels, for simplicity:



(I should confess that I actually used a computer to draw this wavefunction, just to make sure it's accurate. The numerical method that I used is described in the following lesson.)

Now let's think more generally about what an entire solution of the TISE should look like, over the whole range of x. Often, as illustrated in the examples on pages 1 and 4, the classically allowed region is finite so the particle is trapped, with a classically forbidden region to either side. Then, in the classically allowed region, the wavefunction must go through some integer number of half-oscillations or "bumps," separated by zero-crossings or "nodes." The number of bumps (or nodes) must be an integer, so only certain (average) wavelengths are possible, and this implies that the allowed energies are quantized. The one-bump (zero-node) wavefunction will have the longest (average) wavelength and therefore the lowest energy; the two-bump (one-node) wavefunction will have the second-longest (average) wavelength and therefore the second-lowest energy; and so on. To determine the numerical values of these energies, of course, requires doing some actual calculations. Given an energy and the corresponding number of bumps or nodes, however, you should now be able to sketch a qualitatively accurate graph of the wavefunction without doing any calculations at all.

On the other hand, if the classically allowed region extends indefinitely to one side or both, then the wavefunction will go through an infinite number of oscillations, these oscillations can vary continuously in size, and therefore the energies will not be quantized. In general, the energies of a quantum particle are quantized when it is "trapped" but not when it is "free."