The Infinite Square Well

Here is our first potential function. Suppose

$$V(x) = \begin{cases} 0, & 0 \leq x \leq a \\ \infty, & otherwise \end{cases} \quad (1)$$

A particle in this potential is completely free, except at the two ends $x = 0$ and $x = a$, where an infinite force prevents it from escaping. A classical model would be a cart on a frictionless, horizontal air track, with perfectly elastic bumpers–it just keeps bouncing back and forth forever.

Outside this "potential well", $\psi(x) = 0$ (i.e., the probability of finding the particle outside the well is zero). Inside the well, where $V = 0$,[1] the time-independent Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi \quad (2)$$

If we define

$$k \equiv \sqrt{\frac{2mE}{\hbar^2}} \quad (3)$$

then Eq. 2 becomes[2]

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

We recognize this, of course; it is the equation for the undamped, undriven harmonic oscillator, with the familiar solution

$$\psi(x) = A\sin kx + B\cos kx \quad (4)$$

where A and B are the two required arbitrary constants.[3] We find their values, as always, by applying the boundary conditions. Normally, those would be that both ψ and $\frac{d\psi}{dx}$ are continuous; but, since $V \to \infty$ at the boundaries, only the first of these applies.

[1]Please note that $V = 0$ does *not* mean the particle has no energy, or no potential energy; we have simply chosen to define our zero of potential energy to be inside the well (as we are free to do).

[2]Notice that the definition of k implies that $E \geq 0$; this matters, in terms of the work-energy theorem.

[3]Previously we have used the other form of the solution, $\psi(x) = A\cos(kx + \phi)$; however, the form used here gives us more physical insight, especially since the phase angle has no physical significance.

Fortunately, since there are two boundaries, that gives us the required two boundary conditions:

$$\psi(0) = \psi(a) = 0$$

so as to join onto the solution outside the well. Applying the first boundary condition,

$$\psi(0) = 0 = A\sin 0 + B\cos 0 = B$$

so $B = 0$, and hence

$$\psi(x) = A\sin kx$$

Applying the second condition,

$$\psi(a) = 0 = A\sin ka$$

so either $A = 0$ (in which case we are left with the trivial solution $\psi(x) = 0$ everywhere, which is uninteresting[4]), or else $\sin ka = 0$, in which case

$$ka = 0, \pm\pi, \pm 2\pi, \pm 3\pi, \ldots$$

But $ka = 0$ is again trivial, and the negative values give no additional information, so we might as well absorb that minus sign into the constant A. So the distinct solutions require

$$k_n = \frac{n\pi}{a}$$

with $n = 1, 2, 3, \ldots$

However, notice that we have not found the value of A, but rather the value for k (or rather, an infinite number of k_n's), and therefore the possible values for E:

$$E_n = \frac{\hbar^2 k_n^2}{2m} = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{5}$$

And what is E? A quick check of the units is suggestive: E has units of **joules**, that is, units of **energy**. And in fact, E *is* the energy that the particle has, or rather, each E_n (corresponding to a distinct value of n) is the energy of the particle in the well for each possible value for n. Notice that although the particle can have an amount of energy corresponding to (say) $n = 3$, or to $n = 4$, it *cannot* have any energy *between* those two values. The possible energy values for the particle take on *discrete* values, instead of *continuous* ones; we say that the particle's energy is **quantized**.

And if you recall, Planck's hypothesis for blackbody radiation, Einstein's model for the photoelectric effect, and Bohr's model of hydrogen all required the quantization of energy; however, they took it as an ad hoc assumption, without physical basis. Here we see the idea of quantization of energy emerges naturally from the Schrodinger equation.

[4]Actually, we reject $\psi(x) = 0$ it for a far more important and compelling reason; we will get to that soon.

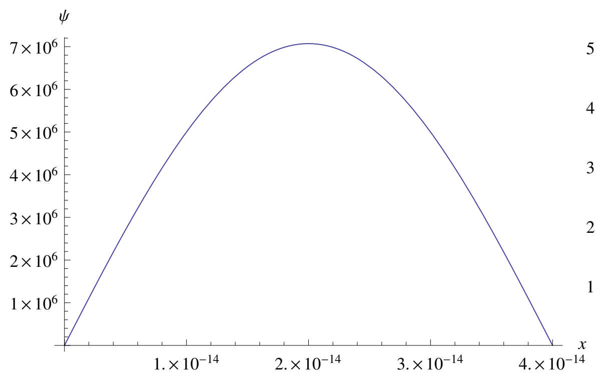
So, how *do* we get the value for A, which we need to complete the solution of Eq. 2? We interpret the wave function <u>physically</u>. Specifically, we recall that $|\Psi(x,t)|^2$ (or, in this case, $|\psi(x)|^2$) represents the probability of the particle being somewhere between x and $x+dx$. Thus, we calculate the probability of the particle being at each possible value of x, and add them. Since the particle has to be *somewhere* inside the well, this sum must be identically 1. The mathematical version of this is, of course,

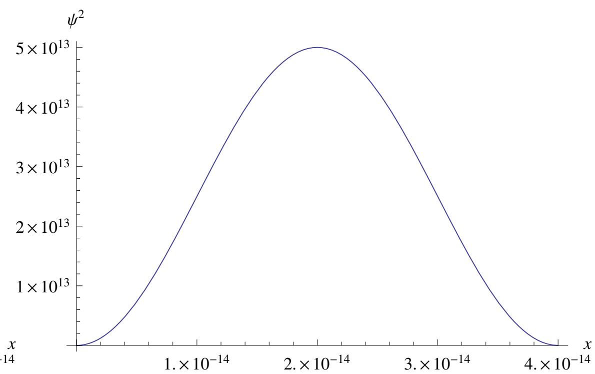
$$\int_0^a |\psi(x)|^2\, dx = \int_0^a |A|^2 \sin^2(kx)\, dx = |A|^2 \frac{a}{2} = 1 \tag{6}$$

so $|A|^2 = \frac{2}{a}$. This only determines the magnitude of A, but the negative root carries no physical significance (trust me!), so we have $A = \sqrt{\frac{2}{a}}$. Inside the well, then, the solutions are

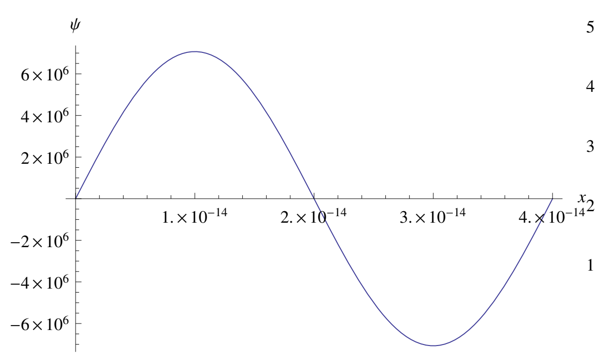
$$\psi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi}{a}x\right) \tag{7}$$

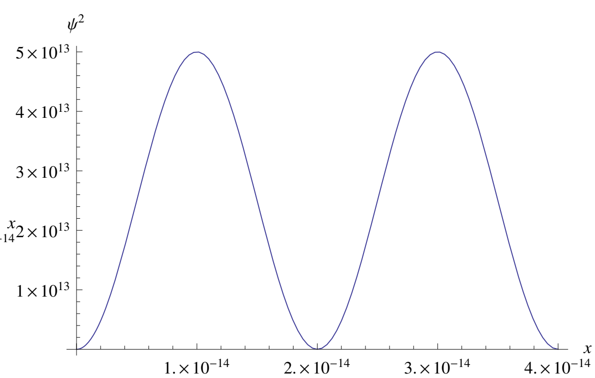
For $n = 1$:



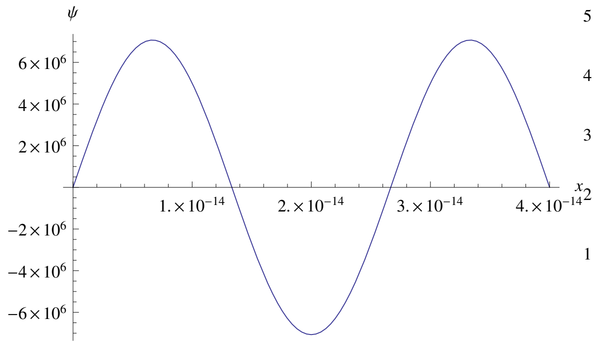


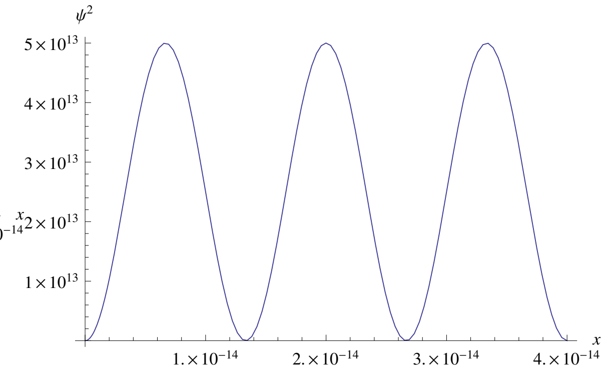
For $n = 2$:





For $n = 3$:





Things to note:

- There is not just *one* solution to this particular system, but an *infinite number*, corresponding to different amounts of (total) energy of the particle, one for each integer n. The first three are plotted above (both ψ and ψ^2).
- The functions $\psi_n(x)$ have the form of a standing wave (t is a fixed value, and so does not appear explicitly).
- The functions ψ_n are alternately even and odd, with respect to the center of the well. (ψ_1 is even, ψ_2 is odd, and so on.)
- Remember that $\psi^2(x)$ represents the probability of the particle being at $x \pm dx$; thus, where the wave function crosses the x axis, the probability of the particle being at that position is *zero*.[5] For example, if the particle has enough energy to be in the $n = 2$ state, the particle cannot ever be at the point in space where $x = \frac{a}{2}$.
- On the other hand, the particle is most likely to be found at those places where ψ^2 is a maximum, e.g., for ψ_1^2, when you take a measurement of the particle's position, the value you are most likely to get is $x = \frac{a}{2}$.

It is for these reasons that physicists often say that a particle has wave-like properties, or that its position is "smeared-out" in space; but please notice that our particle "becomes" a perfectly good particle, with a single, fixed location–*once you determine its location by doing an experiment*.

[5] More precisely, if you make a measurement of the particle's position, you will never find it at those locations where $\psi^2(x) = 0$.