Class Two
Computational Physics

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Last time we learned about finding roots of a function. That is, given a function $f(x)$, we seek the value(s) of x that make $f(x) = 0$. We discussed two methods:

1. Bisection method. This was simple, but slow. Convergence is linear.
2. Newton's method. This was a little more complicated, but much faster. Convergence is quadratic.

Today we will see an example of a problem from physics that requires solving an equation that cannot be solved by hand, and hence requires using a root-finding algorithm. Next week in class and lab we will see how to use matlab's built-in root-finding functions to solve the physics problem for us.

One-dimensional infinite square well. We start with a fairly simple problem from quantum mechanics (QM). This problem can be solved by hand. It will be a warm-up for a more difficult problem that does require a computer. The problem we will consider is that of a single particle in an infinite, square, one-dimensional potential. The potential $V(x)$ is plotted in Fig. 1. You can think of this as a "particle in a box." The infinite potential means that the particle has zero probability of being found outside the box.

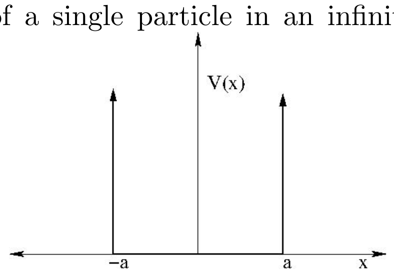

Figure 1: The potential for the infinite square well.

As usual in QM, we start by writing down the Schoödinger equation:

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V(x)\psi(x) \;=\; E\psi(x)\;. \tag{1}$$

In the interior region of the well, $-a \leq x \leq a$, the general solution is:

$$\psi(x) \;=\; A\sin(kx) + B\cos(kx)\;,\ \text{where } k = \sqrt{\frac{2mE}{\hbar^2}}. \tag{2}$$

We will focus on solving for the energies E. We use boundary conditions to solve for A, B, and k. In so doing, we will see that E is quantized; not all energy values are possible.

The wavefunction $\psi(x)$ is zero outside the well, i.e., $\psi(x) = 0$ if $x < -a$ or $x > a$. Since the wavefunction must be continuous, $\psi(x)$ must vanish at the edges of the well. This gives

$$\psi(-a) \;=\; 0 \;\;\Rightarrow\;\;\; -A\sin(ka) + B\cos(ka) = 0\;. \tag{3}$$

$$\psi(-a) \;=\; 0 \;\;\Rightarrow\;\;\; -A\sin(ka) + B\cos(ka) = 0\;. \tag{4}$$

Adding and subtracting these equations yields:

$$B\cos(kx) \;=\; 0\;,\ \text{ and }\ A\sin(ka) \;=\; 0\;. \tag{5}$$

If both A and B are zero, then the above equations are true, but then $\psi(x) = 0$, which is not physically interesting. Instead, we set either A or B equal to zero. If we set $A = 0$, we have:

$$B\cos(kx) \;=\; 0 \quad \Rightarrow \quad ka \;=\; \frac{\pi}{2}, \frac{3\pi}{2}, \cdots, (n+1/2)\pi, \cdots \; . \tag{6}$$

Remembering our expression for k, Eq. (2), we find, after a little bit of algebra, that:

$$E_n \;=\; \frac{(n+1/2)^2\pi^2\hbar^2}{2ma^2} \; . \tag{7}$$

These are the energy value that correspond to even wavefunctions. Similarly, if we set $B = 0$, we find

$$E_n \;=\; \frac{n^2\pi^2\hbar^2}{2ma^2} \; , \tag{8}$$

which correspond to odd wavefunctions. Taken together, Eqs. (7) and (8) specify the allowed energy levels for the infinite square well.

Note that, as usual in QM for bound states, we have found that the energy levels are quantized. Not all energy levels are possible. Note also, however, that there are an infinite number of energy levels; there is no limit to how large n can be in the above two formulas.

hc units. For use later on, let's calculate a numerical value for the ground state of the infinite square well for the case where $a = 0.3$ nm and the particle is an electron. This will also give us practice using "hc" units, which are a very useful set of units that make calculating numbers for atomic physics very easy. The key idea is to measure masses in energy units by multiplying masses by c^2. In so doing, c will appear next to h, so what matters is hc, not h by itself. I would suggest memorizing the following:

$$hc \;=\; 1240\text{eV nm} \quad \text{and} \quad m_e c^2 \;=\; .511\text{MeV} \;=\; 511 \times 10^5\text{eV} \; . \tag{9}$$

If I set $n = 0$ in Eq. (7), multiply top and bottom by c^2, and use the above numbers, I get $E_0 \approx 1.045$ eV for the ground state of the infinite well.

Finite Square Well. We now turn our attention to a more difficult QM problem: The finite square well. Now, instead of an infinite potential for $|x| > a$, the potential has the finite value of V_0. The potential $V(x)$ is illustrated in Fig. 2. Since the potential is finite outside the well, there is a non-zero probability that the particle is found there.

As before, we are mainly interested in the energy levels of the bound states. We shall see that because the well is finite, there are not an infinite number of energy levels.

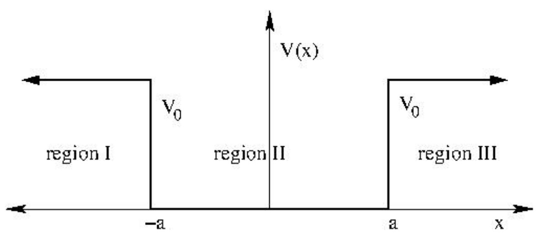

Figure 2: The potential for the finite square well.

To find the energy levels, we need to solve Schrödiner's equation, Eq. (1). There are three different solutions, corresponding to the three regions shown in the figure. The general solution in region I is:

$$\psi_I(x) \;=\; Ce^{\beta x} + De^{-\beta x} \;, \quad \text{where} \quad \beta \;=\; \sqrt{2m(V_o - E)/\hbar^2} \;. \tag{10}$$

The area under $\psi(x)\psi^*(x)$ is a probability. In order for this probability to be normalizable (i.e., finite), it must go to zero as $x \to \infty$. Thus, it must be that $D = 0$. (One can think of this as a "boundary condition" at $x = \infty$.) Hence,

$$\psi_I(x) \;=\; Ce^{\beta x} \;. \tag{11}$$

Similarly, in region III, the wavefunction is given by

$$\psi_{III}(x) \;=\; Fe^{-\beta x} \;. \tag{12}$$

And in region II, we have the same general solution as for the infinite well:

$$\psi_{II}(x) \;=\; A\sin(\alpha x) + B\cos(\alpha x) \;, \text{ where } \alpha = \sqrt{\frac{2mE}{\hbar^2}}. \tag{13}$$

Our task now is to apply boundary conditions. In so doing, we will find the energy levels. In this case, the boundary condition arises from the fact that $\psi(x)$ must be continuous and smooth. This means that the wave functions must have the same value and the same derivative where they meet. $\psi_I(x)$ and $\psi_{II}(x)$ meet at $x = -a$. We thus obtain:

$$\psi_I(-a) \;=\; \psi_{II}(-a) \quad \Rightarrow \quad Ce^{-\beta a} \;=\; -A\sin(\alpha a) + B\cos(\alpha a) \;, \tag{14}$$

$$\psi_I'(-a) \;=\; \psi_{II}(-a) \quad \Rightarrow \quad \beta Ce^{-\beta a} \;=\; A\alpha\sin(\alpha a) + B\alpha\cos(\alpha a) \;, \tag{15}$$

Similarly, requiring that $\psi_{II}(x)$ and $\psi_{III}(x)$, be continuous and smooth at $x = a$ yields:

$$\psi_{II}(a) \;=\; \psi_{III}(a) \quad \Rightarrow \quad Fe^{-\beta a} \;=\; A\sin(\alpha a) + B\cos(\alpha a) \;, \tag{16}$$

$$\psi_{II}'(a) \;=\; \psi_{II}(a) \quad \Rightarrow \quad -\beta Fe^{-\beta a} \;=\; A\alpha\sin(\alpha a) - B\alpha\cos(\alpha a) \;, \tag{17}$$

As before, we have odd and even states, corresponding to $B = 0$ and $A = 0$, respectively. For the even states, $A = 0$. Plugging this in to Eqs. (14)–(17), one obtains:

$$C \;=\; F \;, \quad \text{and} \quad \alpha\tan(\alpha a) \;=\beta \quad \text{(even solutions)} \;. \tag{18}$$

Similarly, if we set $B = 0$, we obtain:

$$C \;=\; -F \;, \quad \text{and} \quad \alpha\cot(\alpha a) \;=-\beta \quad \text{(odd solutions)} \;. \tag{19}$$

A Root-Finding Problem. We have finally arrived at the main result: a problem for which we need a numerical root finder. Eqs. (18) and (19) are both equations that are transcendental; there does not exist an algebraic method to solve them. Numerical methods are thus a necessity.

In the next class we will start with these two equations and discuss how to put them in a form that will be easier for a computer to deal with. In lab, we will then use matlab to solve for the energies of the finite well.