**Class Three**
**Computational Physics**

Dr. David Feldman. December 2011

**Summary of last class: Finite Square Well.** Last time we considered the finite square well, whose potential energy is shown below. We are interested in solving for the allowed energies for the bound states. By solving the Schrödinger equation in the three regions and applying appropriate boundary conditions, we arrived at the following.

$$\alpha \tan(\alpha a) \;=\; \beta \quad \text{(even solutions)} \; . \tag{1}$$

$$\alpha \cot(\alpha a) \;=\; -\beta \quad \text{(odd solutions)} \; . \tag{2}$$

Where,

$$\alpha = \sqrt{\frac{2mE}{\hbar^2}} \;, \quad \text{and}\beta \;=\; \sqrt{2m(V_o - E)/\hbar^2} \; . \tag{3}$$

So we have a fairly complicated set of equations resulting from a fairly complicated mathematical analysis. We will need a computer to solve for the energy levels $E$. How to proceed? Here are some good steps to follow when faced with a situation like this.

**Check limiting cases:** We know that if $v_0 \to \infty$ then we return to the infinite well. As $V_0$ approaches $\infty$, $\beta$ also approaches $\infty$. Thus, Eq. (1) reads $\tan(\alpha a) = \infty$. This will occur when $\alpha a = (n + 1/2)\pi$. You can then show that this yields the energy levels for even states for the infinite well:

$$E \;=\; \frac{(n+1/2)^2\hbar^2\pi^2}{2ma^2} \; . \tag{4}$$

Checking limiting cases is a *very* good idea after you have derived a complicated formula.

**Check for infinities:** Computers do not know what to do when you ask them to divide by zero, or come close to dividing by zero. The tangent function in Eq. (1) is potentially trouble, since $\tan(x)$ goes to infinity. We can get rid of this problem quite easily, by simply re-writing the equation:

$$\alpha \sin(\alpha a) = \beta \cos(\alpha a) \; . \tag{5}$$

There is now no danger of dividing by zero.

For use when we work with matlab, let's re-write this as:

$$\text{even}(E) \;=\; \alpha \sin(\alpha a) - \beta \cos(\alpha a) \; . \tag{6}$$

Thus, we need to find the values of $E$ that make $\text{even}(E)$ equal to zero. (Note that $\alpha$ and $\beta$ are both functions of $E$.) One can also show that Eq. (2) can be written as:

$$\text{odd}(E) \;=\; \alpha \cos(\alpha a) + \beta \sin(\alpha a) \; . \tag{7}$$

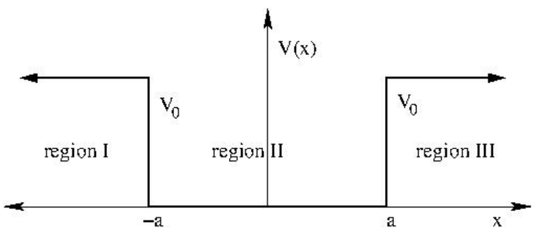


Figure 1: The potential for the finite square well.

**Units:** Before giving these equations to the computer, we need to think about units. We need units such that the numbers the computer will work with are very roughly the same order of magnitude. I like measuring masses in energy units and keeping track of $hc$ instead of $\hbar$. I think these are the easiest units to think in for atomic, molecular, and nuclear physics. Doing so, I can express $\alpha$ and $\beta$ as:

$$\alpha = \sqrt{\frac{8\pi^2 mc^2}{(hc)^2} E} \tag{8}$$

$$\beta = \sqrt{\frac{8\pi^2 mc^2}{(hc)^2} (V_0 - E)} \tag{9}$$

Using the above form for $\alpha$ and $\beta$, we can program even($E$) and odd($E$) into matlab. Once we do so, first make some plots to get a picture of what is going on. Then use the `fzero` function to find numerical values for the zeros. These zeros are the energy levels for the finite square well.

**Assignment Two**
**Computational Physics**
**Kigali Institute of Science and Technology**
December 2011

**This assignment is due at the beginning of class on Thursday, 29 December.**

1. Using the notation from class and the notes, show that if $B = 0$, the allowed energy levels for the infinite square well are
$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{10}$$
2. Using the formulas that we derived in class, find a numerical value for the first three energy levels for the infinite square well for an electron in a well that is 0.3 nm wide. In your carrying out your calculation, use $hc$ units.
3. Fill in the steps between Eqs. (14)–(17) and Eq. (19) from the notes for class two.
4. What is the physical or geometric meaning of $\psi'_{II}(a) = \psi'_{III}(a)$?
5. Explain briefly why is $\psi_{III} = Ee^{\beta x}$ not a physically acceptable solution for the Schödinger Equation in region III of the finite well.