Midterm Exam 03

**Solving an ODE like it’s the Transcontinental Railroad**

When studying the problem of a particle in a finite potential well, we solved for the wave function ψ(x), by integrating a second-order linear differential equation from left-to-right (in position x space) and from right-to-left, iterating over the value of the particle’s energy E until the two integrations match at some prescribed location xmatch. What was different about this particular problem as compared to other ODE problems? Why was it important that we integrate from both directions? Discuss the advantages (and disadvantages) of solving the problem in this way. Can you envision an-other way to solve the problem while still satisfying all of the requirements that originally motivated the two-directional integration solver?

The biggest difference in this problem was although the ODE was like what we had already solved and was quite simple the difference in the finite potential well was the boundary conditions that had to be met. Having boundary conditions turned the ODE problem into an eigenvalue problem that has solutions only for particle values of E or the energy which in our problem was represented as k. We had to integrate from both sides as those were the boundary conditions that we were using. The potential on each side outside the box vanishes to zero exponentially. An advantage to solving the problem this way would be that it is relatively simple. Though I did not understand it very well at first, it is much more general by just solving an ODE solver plus a ‘searcher’ for the lowest eigenvalue which in this case is the most negative energy the particle can have at the bottom of the potential well. This makes it only have a few lines of code and is computationally not very extensive. A potential disadvantage of this method I could see for a problem similar to this would be if you did not know one or both of the boundary conditions. You would then not be able to integrate from both sides. This would also prevent you from find the eigenvalues unless you used a different method. Another slight disadvantage with this method is that using the ODE solver means you solve for the first derivative to then solve for the function though the equation to begin with only relates the function to the second derivative so this method could be computing more than you actually need. A different method for solving this problem is the Numerov Algorithm, which is specialized for ODEs not containing any first derivatives. This method is less general than our previous, but it does provide more precision.

A brief derivation of the method is that you do a Taylor series expansion on the wave function plus some h as well as minus some h ( w(x+h) and w(x-h) ). You then sum these two, drop terms past the fourth derivative and rearrange to solve for the second derivative. Then the fourth derivative is substituted by a derived expression that only depends on the second derivative. Finally using the central-difference approximation for the second derivative you obtain the Numerov algorithm which only uses values of the wave function at the two previous steps x and x-h to move the wave function forward to x + h.

This method only uses the second derivative and does not require the use of specific boundary conditions. However, from looking at the example code in the book, it is more longer and more complicated than our original method which was much more general and easier to understand though again less precise and requiring boundary conditions.