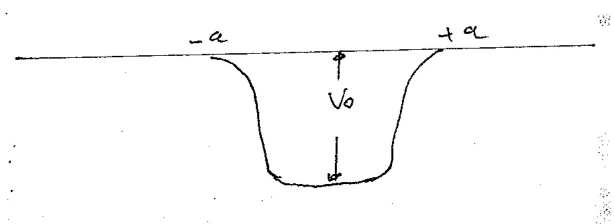
Binding Quantum Particles

ODEs in space variables lead to eigenvalue problems. For instance, think of setting up a standing wave whereby the boundary conditions restrict the wave to be of certain types and to have particular wavelength and frequencies.

To illustrate the solutions of ODEs in space variables, we will look at a particularly simple example from the quantum world. Namely, we will ask whether a nuclear model with nucleons (protons and neutrons) bound in a potential of depth and size comparable to that of a typical nucleus is quantum mechanically consistent and possesses excited states at an energy of several MeV.

The model will consist in placing 1 nucleon (proton or neutron, mass $mc^2 = 940MeV$) in a 1-D potential well of width $a = 2fm$ ($1fm = 10^{13}cm = 10^{-15}m$) and depth $V_0 = 83MeV$. These potential size and depth correspond to the size and interaction strength of a typical nucleus. The 1-D variable x is meant to represent the radial direction. We will then solve for the ground state and exited states of the system.



Quantum Mechanics in a nutshell

Quantum Mechanics is a statistical theory. The probability to find a particle within $dxdydz$ at a position $[x, y, z]$ at the time t is given by $|\psi(x, y, z, t)|^2 dxdydz$. The function $\psi(x, y, z, t)$ is called the *wave function*. It satisfies the *Schrodinger Equation*, a Partial Differential Equation (PDE).

For a bound state, the time dependence is simple and can be taken out. Furthermore, in 1-D the wave function is a function of x only, $\psi(x)$, that satisfies the *1-D time independent Schrodinger equation*.

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

$V(x)$ is the potential, m is the mass of the particle, and $\hbar$ is a constant (the *Planck constant*, with a value such that $\hbar c = 197.32MeV fm$ where c is the speed of light). E is the energy of the bound state. This is an ODE in space variable. It is a *Wave Equation* whose solutions describe standing quantum mechanical wave functions. This is similar to solving for the standing waves on a violin string, but *slightly more challenging mathematically*!

It is convenient to write

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

and to define (E is negative)

$$\kappa^2 = \frac{2m}{\hbar^2}|E|$$

therefore

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}V(x)\psi + \kappa^2\psi$$

The Nuclear Model

Let us consider a finite depth potential of width $-a$ to $+a$, i.e., $V(x) \to 0$ for $x \to \pm\infty$. Therefore, for large $\pm x$ values, Schrodinger equation reduces to

$$\frac{d^2\psi}{dx^2} = \kappa^2\psi$$

The regions outside the well are classically forbidden to the particle (the energy is negative). Quantum mechanics, on the other hand, allows the particle to penetrate in these regions; this is the physical basis for *quantum tunnelling*. Therefore the asymptotic solutions in either sides of the potential well are $\psi(x) \to \exp(-\kappa x)$ for large positive x and $\psi(x) \to \exp(\kappa x)$ for large negative x. These are the two boundary conditions that $\psi(x)$ must satisfy.

The wave function $\psi(x)$ is a solution of a second order ODE. Therefore it must be continuous for all x, both inside and outside of the potential well. Together with the two boundary conditions described above, this requirement restricts the allowed solution to very specific standing wave shapes.

The energy E, or κ, is the quantity labeling the allowed states. In other words, only particular values of E allow a solution $\psi(x)$ to satisfy the 2nd order Schrodinger equation (ODE) simultaneously with the boundary conditions. E is the *quantized* energy. It may take one or many values. The *1-D time independent Schrodinger equation* is said to be an eigenvalue problem.

RK4 Solution

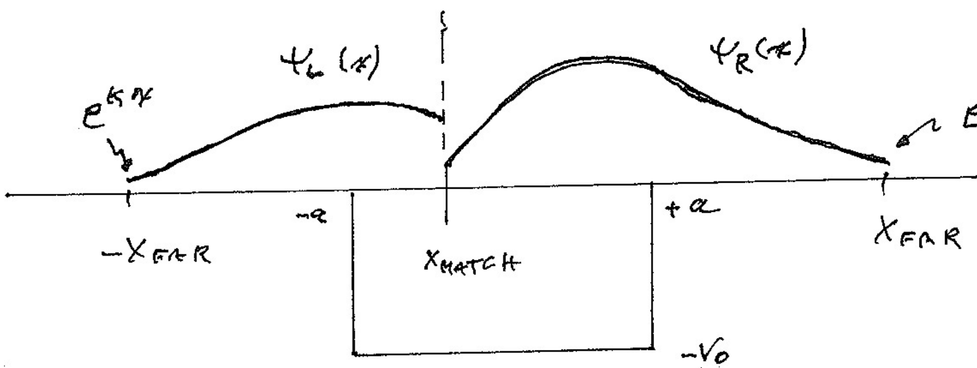
We want to solve the 1-D Schrodinger equation via the RK4 method. To do so, rewrite it in a canonical form

$$\frac{d\psi}{dx} = \chi$$

$$\frac{d\chi}{dx} = \frac{2m}{\hbar^2}V(x)\psi + \kappa^2\psi$$

The auxiliary function $\chi(x)$ will be solved for simultaneously with the wave function $\psi(x)$.

Details of the Solution



- Starting at $x = -Xfar$, use RK4 to integrate toward the right from $x = -Xfar$ to $x = Xmatch$, starting from the asymptotic negative x solution.

  $Xfar$ is an arbitrary far distance, outside the well, where $\psi(x)$ takes its asymptotic form. $Xmatch$ is the point at which the solution from the left and from the right will be matched.

  Use $Nsteps$ x steps in this RK4 solution and the one from the right (next).

- Starting at $x = +Xfar$, use RK4 to integrate toward the left from $x = +Xfar$ to $x = Xmatch$, starting from the asymptotic positive x solution.

- At $x = Xmatch$, the wave function must be continuous, i.e., $\psi(x)$ and $\chi(x)$ must be continuous.

  Calculate a function $W(E)$ which depends on the energy

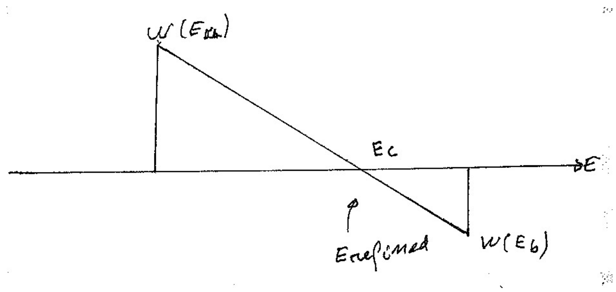
$$W(E) = \frac{\frac{\psi_L'}{\psi_L} - \frac{\psi_R'}{\psi_R}}{\frac{\psi_L'}{\psi_L} + \frac{\psi_R'}{\psi_R}}$$

  The use of the logarithmic derivative $\frac{\psi'}{\psi}$ in $W(E)$ is to avoid problems with the norm (multiplicative constant) of $\psi(x)$. The denominator is to avoid small and large numbers. Allowed values of E will be such that $W(E) = 0$.

- Search for proper E. This can be done by the following procedure.

  - Scan over a lattice in E spanning a range $E = [-0.95V_0, 0]$. Use a scanning step $descan$.

- Find a change in sign in $W(E)$
- Use a bisection step two times to refine the solution twice, i.e.,



- Repeat for every bound state.

- For each bound state energy found above, solve again for $\psi_L x)$ and $\psi_R(x)$. Store the wave function in an array. At the matching point adjust $\psi_R(x)$ so that $\psi_R(Xmatch) = \psi_L(Xmatch)$. This should yield a continuous wave function. Plot it as a check.

- If $|\psi(x)|^2 dx$ is the probability to find the particle in the interval dx centered on x, then the wave function must be *normalized*, i.e.,

$$\int_{-\infty}^{\infty} \psi(x)^2 dx = 1$$

  must be required. This says that the particle must be somewhere!

  The wave function obtained so far is unlikely to be normalized. This must now be imposed numerically:

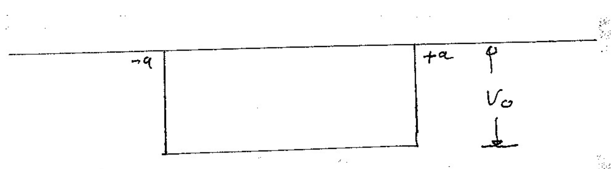
  - Use the trapezoidal rule to calculate the area under $\psi(x)^2$; call it NORM.
  - Normalize $\psi(x)$, i.e., calculate $\frac{1}{\sqrt{NORM}}\psi(x)$.

- Find all bound states and plot the corresponding normalized wave functions

- Comment on the symmetry of wave functions and their energies.

1-D Square Well Potential

The method of solution explained above is general and can solve any model harboring any local 1-D potential. However, to answer the qualitative question posed earlier, it is sufficient to use a simple symmetric square well potential, $V(x) = -V_0$ for $|x| <= a$ and $V(x) = 0$ otherwise.



Schrodinger equation then becomes

$$\frac{d^2\psi}{dx^2} = -\frac{2m}{\hbar^2}V_0\psi + \kappa^2\psi$$

inside the well, and

$$\frac{d^2\psi}{dx^2} = +\kappa^2\psi$$

outside the well.

Constants

Use $V_0 = 83MeV$, $a = 2fm$, $Xfar = 6fm$, $Xmatch = -0.5fm$.
Use $Nsteps = 150$.
Use $descan = 0.5$ to scan the energy range.
Use $\frac{2m}{\hbar^2} = \frac{2mc^2}{(\hbar c)^2} = \frac{2\ 940MeV}{(197.32MeVfm)^2} = 0.0483\ MeV^{-1}fm^{-2}$.

Ref: R. Landau, M. J. Paez and C. C. Bordeianu,
A Survey of Computational Physics,
Princeton University Press, 2008