1 Numerov's algorithm

The aim of this project is to solve the time-independent Schrödinger equation for a potential $V(x)$ as given by

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

Not every potential can be solved analytically, but it is possible to use a numerical method. In this case we choose to use Numerov's method which can be used to solve second order differential equations of the form

$$\frac{d^2y}{dx^2} + k(x)y(x) = 0, \tag{2}$$

where in our case

$$k(x) = \frac{2m}{\hbar^2}(E - mV(x)). \tag{3}$$

Numerov's method discretizes a taylor series for $\psi(x+dx)$ into $x_n = x_0 + ndx$ and preserves any terms up to $O(dx^6)$ to work out the second derivative in the Schrödinger equation. This leads to a discretized wavefunction of the form

$$\psi_n = \frac{2\big(1 - \frac{5}{12}dx^2k_{n-1}^2\big)\psi_{n-1} - \big(1 + \frac{1}{12}dx^2k_{n-2}^2\big)\psi_{n-2}}{1 + \frac{1}{12}dx^2k_n^2}, \tag{4}$$

which can be evaluated numerically on a grid x_n, given two initial guesses ψ_0 and ψ_1.

The goal of this method is to find the correct energy eigenvalues. We know that we have obtained a correct energy whenever the corresponding wavefunction has the properties

- $\int_{-\infty}^{\infty} |\psi(x)|^2 = 1$
- $\psi(x) \to 0$ as $x \to \pm\infty$
- $\psi(x)$ and $\psi'(x)$ are continuous.

Of course it is impossible to use an infinite grid in a simulation, therefore we will make use of the fact that the wavefunction decays exponentially to zero in the classically forbidden regime where $E < V(x)$ and construct the grid $[x_{min}, x_{min+1}, ..., x_{max}]$ such that x_{min} and x_{max} are deep within this forbidden regime. The initial guess for the wavefunction is then chosen to be $\psi_0 = 0$ and $\psi_1 =$ *some small constant*.

One problem however is that a second solution exists where ψ diverges to $\pm\infty$ within the classically forbidden regime. The simulation cannot distinguish between the correct and incorrect solutions and the slightest numerical imprecision will lead then to rapid divergence of the solution. To fix this problem we perform the Numerov integration twice. First from left to right on the grid up to a matching point x_{match}, then from right to left on the grid up to the matching point. Commonly the matching point is chosen to be the rightmost classical turning point such that $V(x_{cl} - dx) < E$ and $V(x_{cl} + dx) > E$. We can then ensure that

$$\psi_{left}(x_{cl}) = \psi_{right}(x_{cl}) \tag{5}$$

$$\left.\frac{d\psi_{fwd}}{dx}\right|_{x_{cl}} = \left.\frac{d\psi_{bwd}}{dx}\right|_{x_{cl}}. \tag{6}$$

Within the discretized Numerov method the discontinuity at the classical turning point can be approximated by

$$\psi'_{icl} - \psi'_{icl} = \frac{\psi_{icl-1} + \psi_{icl+1} - (2 - k_{icl}dx^2)\psi_{icl}}{dx} \tag{7}$$

and when its value is close to zero the wavefunction also obeys the normalization and continuity requirements.

When the wavefunction indeed satisfies all requirements we know that the corresponding energy is an eigenvalue of the Schrödinger equation. In order to find the desired energy levels we use can make use of the fact that the number of nodes, n, corresponds to the nth excited state. Therefore, when we want to find the ground state and first excited state of the system we have to find the solutions that have 0 and 1 node(s) respectively. The energy levels can be found using a bisection algorithm:

- Start by choosing an energy range (E_{min}, E_{max}) and make an initial guess $E_{guess} = \frac{E_{max}+E_{min}}{2}$.
- Choose x_{min} and x_{max} deep within the classically forbidden regime for this E_{guess} and calculate ψ_{fwd} from x_{min} up to the last classical turning point x_{cl}.
- Calculate ψ_{bwd} from x_{max} up to the last classical turning point x_{cl}.
- Scale $\psi_{bwd}(x_{cl})$ by a factor $\psi_{fwd}(x_{cl})/\psi_{bwd}(x_{cl})$ to ensure that $\psi_{fwd}(x_{cl}) = \psi_{bwd}(x_{cl})$ and paste them together to obtain $\psi(x_i)$.
- Calculate the number of nodes, n, i.e. find the number of times $\psi(x_i)$ crosses zero.
- If $n >$ the desired number of nodes set $E_{max} = E_{guess}$ and start again. If $n <$ the desired number of nodes set $E_{min} = E_{guess}$ and start again.
- If n is the desired number of nodes calculate the discontinuity $\psi'_{icl} - \psi'_{icl}$. If the discontinuity is > 0 set $E_{max} = E_{guess}$ and if it iss < 0 set $E_{min} = E_{guess}$ and start again.
- After several iterations the absolute value of the discontinuity will be smaller than a certain threshold. This means that the wavefunction is proper and that the E_{guess} has converged to the desired energy eigenvalue.

This bisection algorithm combined with Numerov's method gives a solid method to calculate bound states of the Schrödinger equation numerically for arbitrary potentials. Its correctness is easily verified by applying the algorithm to the quantum harmonic oscillator for which the energy eigenvalues are analytically known to be $\hbar\omega(n + \frac{1}{2})$.