Numerical Integration of the Schrödinger equation by a Finite Difference Method

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1 Description of the method

We wish to obtain numerically the energy levels (eigenvalues) E and stationary states (eigenfunctions) $\Psi(x)$ of the one-dimensional Schroedinger equation for a particle of mass m in a potential $V(x)$:

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

The method, proposed by D. Truhlar [1], is based on replacing the derivative appearing in Eq.(1) by finite differences. The concept of numerical derivation by finite difference is summarized in Figure 1. The domain is divided into a finite

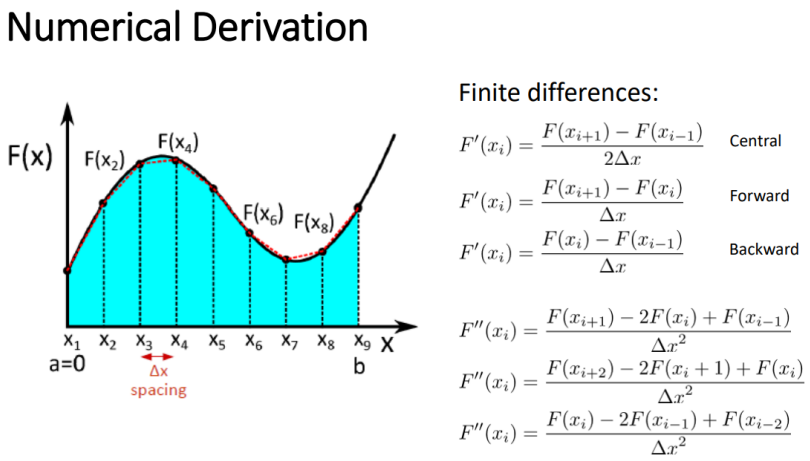

Figure 1: Calculation of first and second derivatives of a function $F(x)$ using finite elements.

set of points $(x_1, ...x_N)$ with a separation Δx. The function $F(x)$ is evaluated at

these points obtaining $F(x_1), ..., F(x_N)$. From these values, the first derivative and second derivatives of F can be calculated at the points by replacing the derivatives by differences (note that, as shown in Figure 1, there are several different possibilities for the numerical calculation of these derivatives).

2 Implementation

The first step to implement this algorithm is to select an appropriate system of units, in which all calcualtions will have a reasonable order of magnitude (it is not reasonable to ask the computer to perform calculations with very large and very small numbers).

As in the original reference, we note that once the system of units has been selected, Eq.(1) can be expressed as:

$$-\frac{1}{2\mu}\frac{d^2}{dx^2}\Psi(x) + V(x)\Psi(x) = E\Psi, \tag{2}$$

being μ a constant that depends on the chosen system of units. Now, we divide the domain into a finite number N of points x_i with a separation $h = \Delta x$ and we denote by Ψ_i and V_i the values of the wavefunction and the potential evaluated at x_i. Using Figure 1, we can express the second derivative appearing in Eq.(2) as follows:

$$\left.\frac{d^2}{dx^2}\Psi(x)\right|_{x=x_i} \approx \frac{\Psi_{i-1} - 2\Psi_i + \Psi_{i+1}}{h^2}. \tag{3}$$

Using Eq.(3) in (2) we obtain:

$$\frac{1}{\mu}\Psi_{i-1} + \left[-\frac{2}{\mu} - 2h^2V_i\right]\Psi_i + \frac{1}{\mu}\Psi_{i+1} = -2h^2E\Psi_i. \tag{4}$$

As a boundary condition, we have to impose that Ψ is zero at the extreme points of the domain (x_1 and x_N), so we have $\Psi_1 = 0$ and $\Psi_N = 0$.

Now, the problem of solving a differential equation has been transformed to the problem of solving Eq. (4) which is lineal algebra problem of the diagonalization of a matrix. As a result, the diagonalization process gives the possible values of E and the wavefunction corresponding to each energy value E evaluated at all the domain. That diagonalization problem can be easily implemented in Python using Numpy.

References

[1] D. G. Truhlar. Finite difference boundary value method for solving one-dimensional eigenvalue equations. *Journal of Computational Physics*, 10(1):123–132, 1972.