

Collocation method with B-splines

for Solving Poisson's Equation in Spherical Symmetry

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1 Introduction

In this assignment, we use the B-spline collocation method to solve Poisson's equation for spherically symmetric systems applied for different one-dimensional charge distributions. In particular, we consider the potential arising from a uniformly charged sphere, a uniformly charged shell, and the electron charge distribution of the hydrogen atom in its ground state.

2 Theory

2.1 Poisson's Equation in Spherical Coordinates

In spherical coordinates, Poisson's equation writes (assuming only radial dependence):

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dV}{dr} \right) = -4\pi\rho(r), \quad (1)$$

Using the help function $V(r) = \phi(r)/r$ and some rearranging gives us:

$$\frac{d^2\phi}{dr^2} = -4\pi r \rho(r). \quad (2)$$

We now solve a second-order differential equation for $\phi(r)$.

2.2 Charge Distributions

2.2.1 Uniformly Charged Sphere

For a sphere of radius R where the total charge Q is uniformly distributed, the charge distribution is given by:

$$\rho(r) = \begin{cases} \frac{Q}{V} = \frac{3Q}{4\pi R^3} & \text{for } r \leq R \\ 0 & \text{for } r > R \end{cases} \quad (3)$$

The analytical expression for the potential is:

$$V(r) = \begin{cases} \frac{Q}{2R} \left(3 - \frac{r^2}{R^2} \right) & \text{for } r \leq R \\ \frac{Q}{r} & \text{for } r > R \end{cases} \quad (4)$$

2.2.2 Uniformly Charged Shell

Similarly, for a shell with inner radius, R_{inner} , and outer radius, R_{outer} , where the total charge Q is uniformly distributed, the charge distribution is given by:

$$\rho(r) = \begin{cases} 0 & r < R_{inner} \\ \frac{Q}{V} = \frac{3Q}{4\pi(R_{outer}^3 - R_{inner}^3)} & R_{inner} \leq r \leq R_{outer} \\ 0 & r > R_{outer} \end{cases} \quad (5)$$

The analytical potential is:

$$V(r) = \begin{cases} \frac{3Q}{2(R_{outer}^3 - R_{inner}^3)} (R_{outer}^2 - R_{inner}^2) & r < R_{inner} \\ \frac{3Q}{(R_{outer}^3 - R_{inner}^3)} \left(\frac{R_{outer}^2}{2} - \frac{1}{3} \left(\frac{R_{inner}^3}{r} + \frac{r^2}{2} \right) \right) & R_{inner} \leq r \leq R_{outer} \\ \frac{Q}{r} & r > R_{outer} \end{cases} \quad (6)$$

2.2.3 Hydrogen Ground State

The electron charge distribution in the ground state of the hydrogen atom is given by:

$$\rho(r) = \frac{1}{\pi} e^{-2r} \quad (7)$$

The corresponding potential is given by:

$$V(r) = \frac{1}{r} - e^{-2r} \left(\frac{1}{r} + 1 \right) \quad (8)$$

3 Numerical Method

3.1 Collocation method with B-Splines

To approach this problem numerically, we will use a collocation method based on B-spline basis functions. Given a knot sequence, we construct B-spline basis functions $B_i(r)$ of order $k = 4$, along with their second derivatives $B''_i(r)$, using recursive algorithms.

We discretized the domain with a set of collocation points r_j , the function $\phi(r)$ can now be approximated as:

$$\phi(r_i) \approx \sum_{n=i-k+1}^{i-1} c_n B_{n,k}(r_i). \quad (9)$$

where x_k is our first physical knot point. At each collocation point, we enforce the differential equation:

$$\sum_i c_i B''_i(r_j) = -4\pi r_j \rho(r_j). \quad (10)$$

Which land us in the linear system:

$$A\vec{c} = \vec{b} \quad (11)$$

where $A_{ji} = B''_i(r_j)$, $B_i = -4\pi r_i \rho(r_i)$ and C_i are the coefficients we want to solve for, we then compute the potential along the defined grid with N points.

To match the number of equations with the number of unknowns, we apply the following boundary conditions:

$$\begin{aligned} V(0) &= 0 \\ V\left(\lim_{r \rightarrow \infty}\right) &= Q \end{aligned}$$

Finally, in order to handle the discontinuities in $\rho(r)$ accurately, the knot sequence is constructed by clustering knots around discontinuity points.

3.2 Limitations of the Model

Although our method gives reliable numerical solutions for Poisson's equation in spherical symmetry, a few limitations should be noted.

3.2.1 Numerical limitations

Knot placement The placement and density of the knots affect the accuracy and stability of the numerical solution. Too few or poorly placed knots can miss key features in regions with discontinuities, while too many can lead to ill-conditioned matrices.

Boundary conditions The results are highly sensitive to where boundary conditions are applied, especially near the edges of the computational domain. This can lead to slight mismatches as seen in the shell potential case.

4 Results

4.1 Uniformly Charged Sphere

Figure 1 shows the numerical and analytical potentials for a uniformly charged sphere:

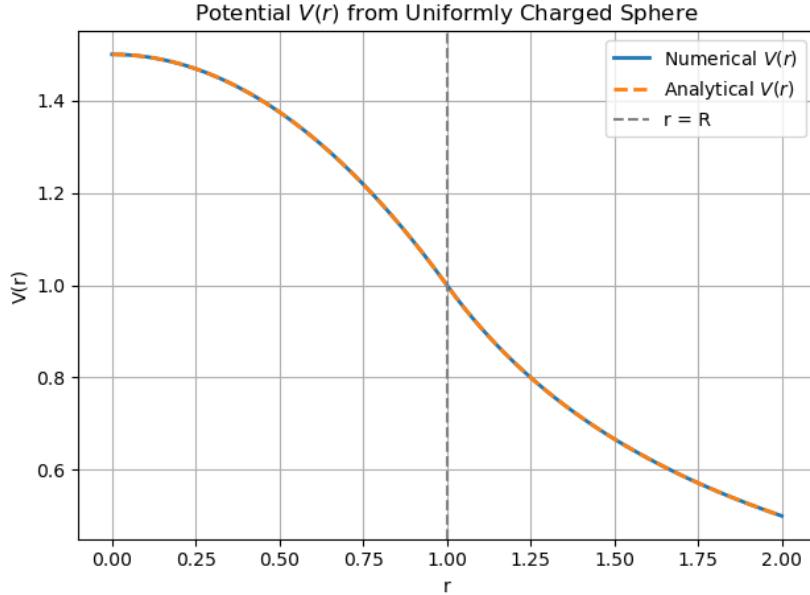


Figure 1: Numerical and analytical solutions for a uniformly charged sphere.

The results match perfectly across the entire domain, the potential inside the sphere behaves quadratically as expected, to then transition smoothly to Coulomb potential outside the sphere.

4.2 Uniformly Charged Shell

Similarly, Figure 2 shows the numerical and analytical solutions for the uniformly charged shell:

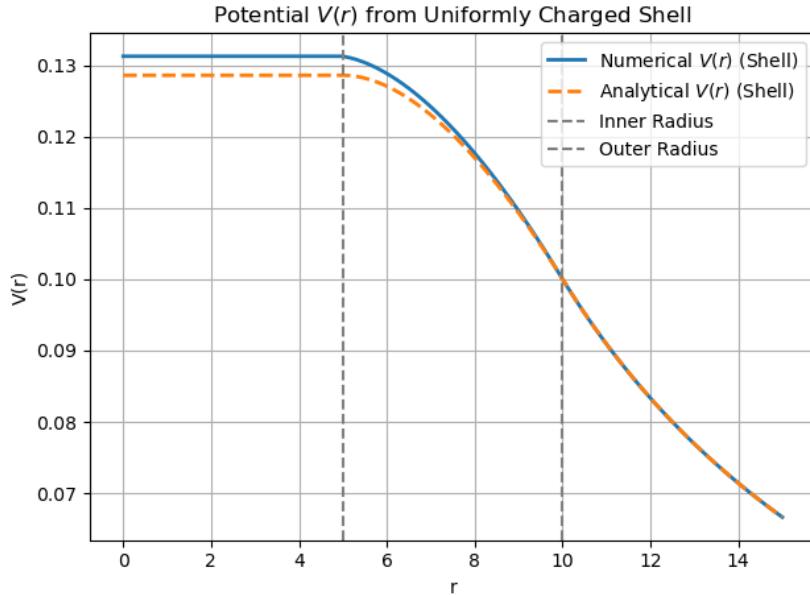


Figure 2: Numerical and analytical solution for the uniformly charged shell.

We observe that the numerical solution closely follows the analytical potential, it is constant inside the inner radius, decaying inside the shell region, and finally matches the Coulomb potential beyond the outer radius.

The B-spline again successfully captures the discontinuities in the derivatives around the shell boundaries. However there is a slight mismatch at small r , which can be attributed to the limitations discussed in 3.2.

4.3 Hydrogen Ground State

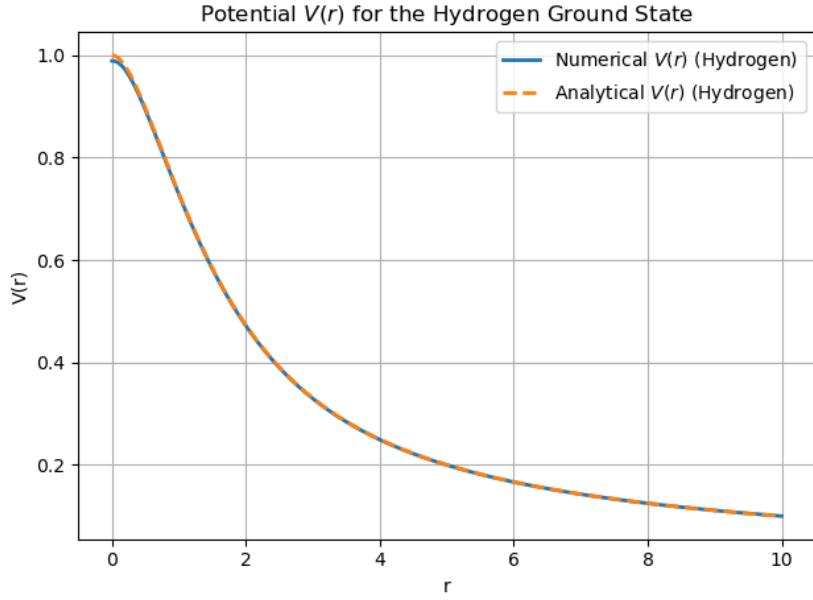


Figure 3: Numerical and analytical potential from the hydrogen ground state density.

In the case of the electron charge density for the Hydrogen ground state wave function, we can see in Figure 3 that the two curves overlap almost perfectly, capturing the exponential decay and the maxima at $r \approx 1$ ¹, since the electron cloud is most dense near the nucleus and decays exponentially with distance.

5 Discussion

The numerical results shows good agreement with the analytical solutions for all different charge distributions. The B-spline collocation method has proven effective for solving Poisson's equation in spherical symmetry for both classical and quantum systems.

¹corresponding to the Bohr radius in atomic units