

Solving the spherically symmetric Poisson equation using B splines Method

Introduction

Poisson's equation is given by

$$\nabla^2 \varphi = -\rho/\epsilon_0 \quad (1)$$

where φ is the electric potential, ρ is a charge distribution and ϵ_0 is the permittivity of free space. For a spherically symmetric problem, the equation simplifies to

$$\frac{d^2 \varphi}{dr^2} + \frac{2}{r} \frac{d\varphi}{dr} = -\rho(r)/\epsilon_0 \quad (2)$$

and by defining the function $u = r\varphi$, this becomes

$$\frac{d^2 u}{dr^2} + r\rho(r)/\epsilon_0 = 0. \quad (3)$$

A description will now be given on how this equation was solved numerically using B-splines for the following charge distributions:

1. A uniformly charged sphere,

$$\rho(r) = \begin{cases} 3q/(4\pi R^3), & r \leq R \\ 0, & r > R \end{cases} \quad (4)$$

where q is the total charge and R is the radius of the sphere.

2. A uniformly charged shell,

$$\rho(r) = \begin{cases} 0, & r < R_1 \\ 3q/(4\pi(R_2^3 - R_1^3)), & R_1 \leq r \leq R_2 \\ 0, & r > R_2 \end{cases} \quad (5)$$

where R_1 and R_2 are the inner and outer radii, respectively.

3. The electron charge distribution in an hydrogen atom:

$$\begin{aligned} \rho_{1s}(r) &= \frac{q}{\pi a_0^3} e^{-2r/a_0} \\ \rho_{2s}(r) &= \frac{q}{32\pi a_0^3} \left(2 - \frac{r}{a_0}\right)^2 e^{-r/a_0} \\ \rho_{3s}(r) &= \frac{q}{3 \cdot 81^2 \pi a_0^3} \left(27 - 18\frac{r}{a_0} + \frac{r^2}{a_0^2}\right)^2 e^{-2r/3a_0} \end{aligned} \quad (6)$$

where a_0 is the Bohr radius.

Since $\varphi(r) = u(r)/r$ and we wish $\varphi(0)$ to be finite, we let $u(0) = 0$. For the first and second charge distributions, we know that $u(r) = q/4\pi\epsilon_0$ outside the enclosing volumes because of Gauss's law. Accordingly, we let $u(R) = q/4\pi\epsilon_0$ for the first distribution and $u(R_2) = q/4\pi\epsilon_0$ for the second distribution. For the third distribution, we introduce a cut-off so that $u(\alpha a_0) = q/4\pi\epsilon_0$ where α is some constant which will later be determined such that the error from this approximation becomes negligible. To facilitate the numerical calculations, the following dimensionless variables were defined:

$$\begin{aligned} \xi &= r/r_0 \\ \lambda &= u/(q/4\pi\epsilon_0) \end{aligned} \quad (7)$$

where r_0 is equal to R for the first distribution, R_2 for the second distribution and αa_0 for the third distribution. Then equation (3) can be written as

$$\lambda''(\xi) + \xi\sigma(\xi) = 0 \quad (8)$$

where $\sigma = 4\pi r_0^3 \rho/q$. The boundary conditions for λ are $\lambda(0) = 0$ and $\lambda(1) = 1$. Defining a new function, $g(\xi) = \lambda(\xi) - \xi$, we obtain the following boundary value problems:

$$\begin{aligned} g''(\xi) + \xi\sigma(\xi) &= 0 \\ g(0) &= g(1) = 0. \end{aligned} \quad (9)$$

These are the equations that were solved for the different charge distributions, σ .

To do so, a collocation method with B-splines as candidate solutions was used. The numerical solution to g was written as

$$\hat{g}(\xi) = \sum_{j=0}^{n-1} c_j B_{j,k}(\xi) \quad (10)$$

where $B_{j,k}$ are B-splines of order $k = 3$. Four knot points were placed at $\xi = 0$ and another four at $\xi = 1$ so that the only non-zero B-spline at $\xi = 0$ was $B_{1,k}$ and the only non-zero B-spline at $\xi = 1$ was $B_{n,k}$. The boundary conditions were thus satisfied by setting $c_1 = c_{n-1} = 0$. The other knot points, as well as the collocation points ξ_k , were evenly spaced on $(0, 1)$. The coefficients were then obtained by solving the linear system of equations:

$$\begin{aligned} c_0 &= 0, \quad c_{n-1} = 0, \\ \sum_{j=0}^{n-1} c_j B''_{j,k}(\xi_k) + \xi_k \sigma(\xi_k) &= 0, \quad k = 1, 2, \dots, n-2. \end{aligned} \quad (11)$$

Results

The results for the first charge distribution can be seen in figures 1 and 2. In the first figure, the B-spline approximation \hat{g} to the boundary value problem (9) is plotted along with the B-splines used and the exact solution g which can be obtained by integrating (9) twice. The B-spline approximation was compared to the exact solution and it was found that even for a small number of B-splines (< 10), the errors in the collocation points were vanishingly small. In the second figure, the electric potential and electric field, (which was obtained by numerically differentiating the potential), are plotted. A similar plot for the second charge distribution is shown in figure 3 and the same for the hydrogen charge distributions in figures 4 and 5.

The parameter α , which determined the length

scale for the hydrogen distributions, was chosen such that the electric field satisfied $E \approx q/(4\pi\epsilon_0 x^2 a_0^2)$ for $x \geq \alpha$. For the 1s, 2s and 3s distributions, it proved sufficient to let $\alpha = 25$.

The maximum error of $|g - \hat{g}|$ in the collocation points as a function of the number of splines is plotted in figure 6.

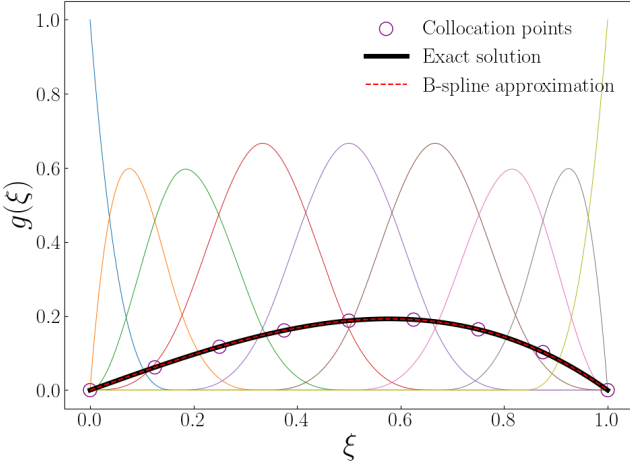


Figure 1: The solution to the boundary value problem given in equation (9) for the uniformly charged sphere. Nine B-splines were used (plotted in background) for which the coefficients were $\mathbf{c} = (0, 0.028, 0.08, 0.15, 0.19, 0.19, 0.14, 0.056, 0)$.

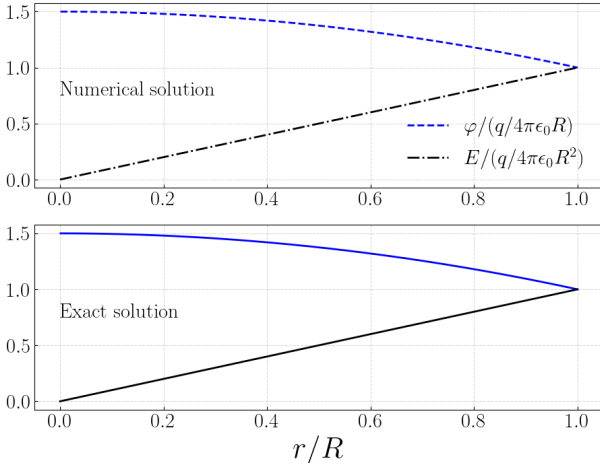


Figure 2: The potential and electric field inside a uniformly charged sphere.

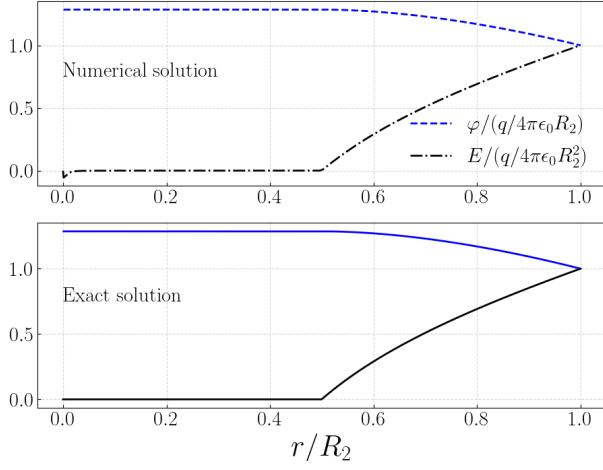


Figure 3: The electric potential and field inside a shell with inner and outer radii ratio $r_1/r_2 = 0.5$. the number of b-splines was 84 and the maximum error in the collocation points was $\approx 2 \cdot 10^{-5}$.

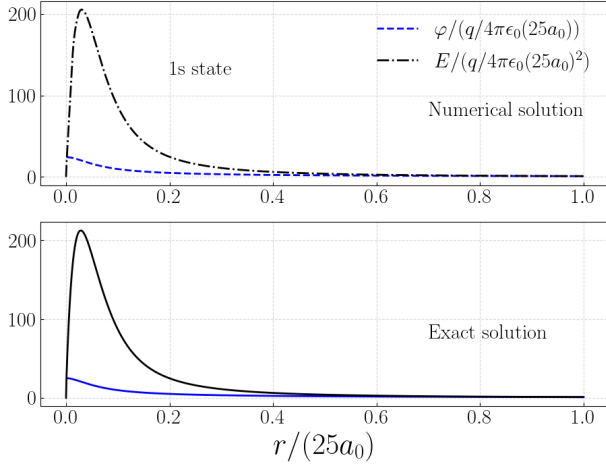


Figure 4: The electric potential and field of the electron charge distribution of a hydrogen atom. the number of b-splines was 84 and the maximum error in the collocation points was $\approx 3 \cdot 10^{-3}$.

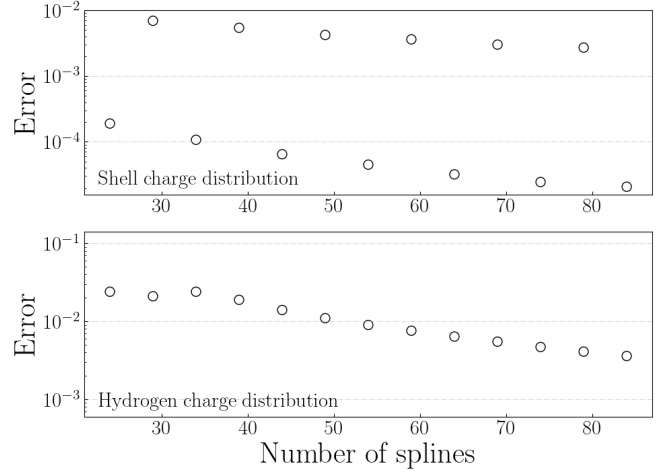


Figure 6

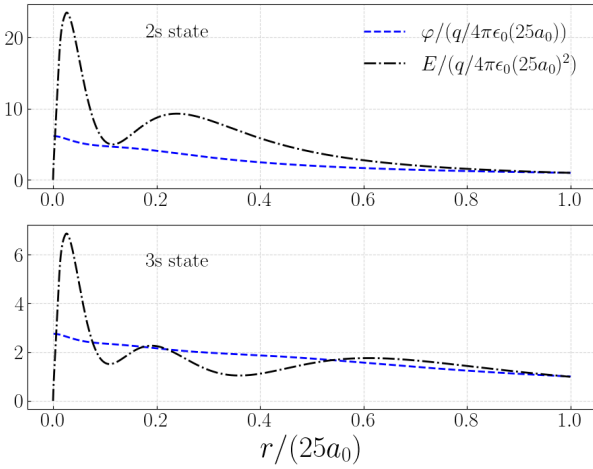


Figure 5: The maximum errors in the collocation points of the shell and hydrogen charge distributions when using the B-spline approximation.