Solving the spherically symmetric Poisson equation using B-splines

Introduction

Poisson's equation is given by

$$\nabla^2 \varphi = -\rho/\epsilon_0 \tag{1}$$

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

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

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

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

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

1. A uniformily charged sphere,

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

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

2. A uniformily charged shell,

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

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

3. The electron charge distribution in an hydrogen atom:

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

   where a_0 is the Bohr radius.

Method

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 type of 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 negliable. To facilitate the numerical caluclations, the following dimensionless variables were defined:

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

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

$$\lambda''(\xi) + \xi\sigma(\xi) = 0 \tag{8}$$

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:

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

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

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

where $B_{j,k}$ are B-splines of degree $k = 3$. 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:

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

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.

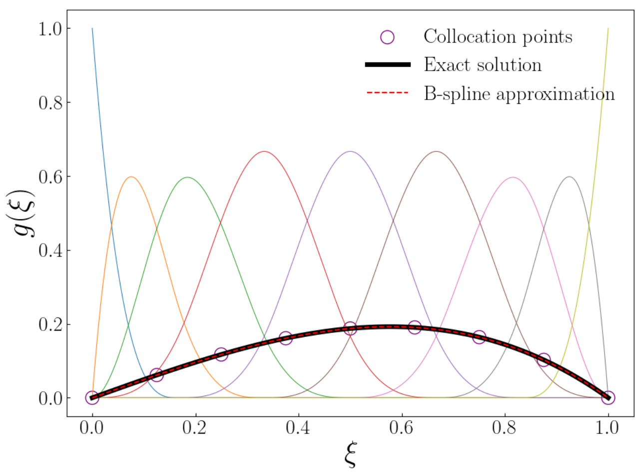

Figure 1: The solution to the boundary value problem given in equation (9) for the uniformily charged sphere. Nine B-splines were used (plotted in background) for which the coefficients were $\mathbf{c} = (0, 0.028, 0.08, 0.15, 0.19, 0.19, 0.14, 0.056, 0)$.

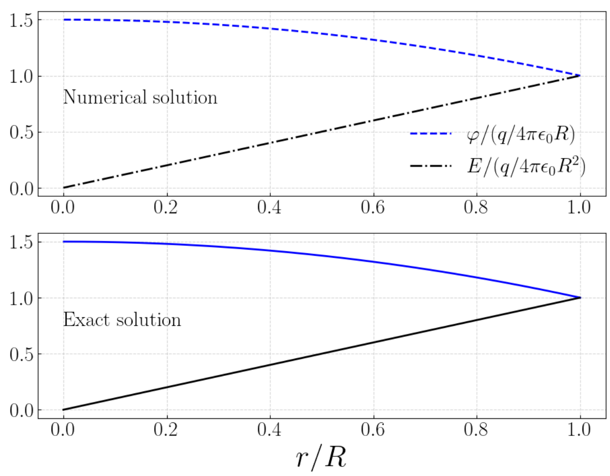

Figure 2: The potential and electric field inside a uniformily charged sphere using B-splines (top) compared to the real solution (bottom).

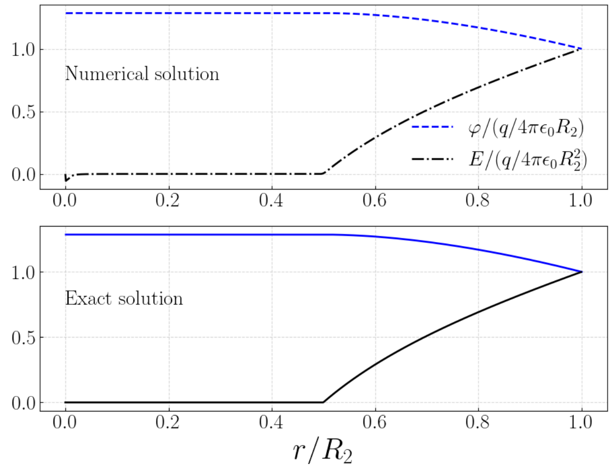

Figure 3: The electric potential and field inside a shell with inner and outer radii ratio $R_1/R_2 = 0.5$. The number of B-splines was 84 and the maximum error in the collocation points was $\approx 2 \cdot 10^{-5}$.

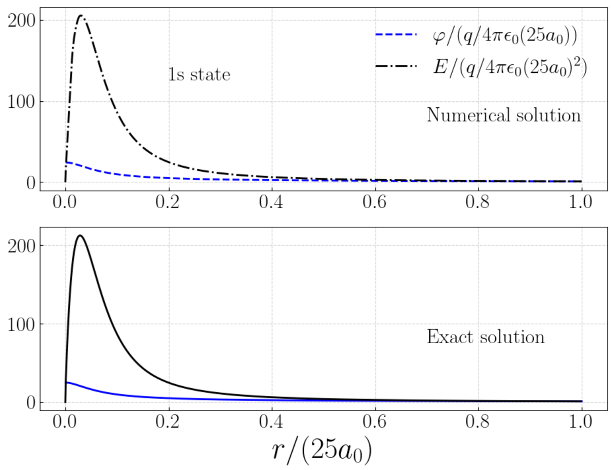

Figure 4: The electric potential and field of the electron charge distribution of a hydrogen atom in 1s state. The number of B-splines was 84 and the maximum error in the collocation points was $\approx 3 \cdot 10^{-3}$.

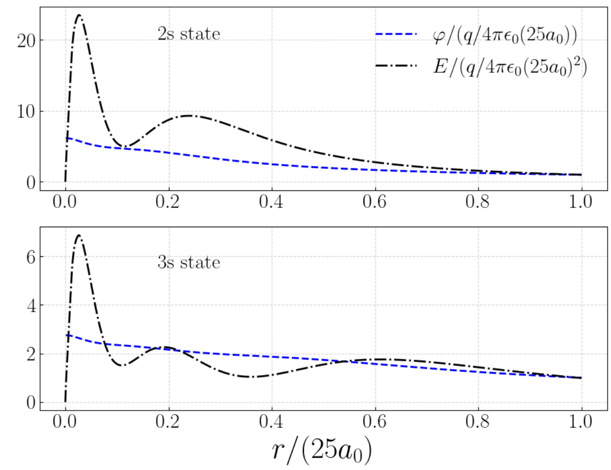

Figure 5: The potential and electric field from the electron charge distributions of the 1s and 2s states of hydrogen atom.

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 the boundary value problem (9) in the collocation points, i.e. $\max|g(\xi_k) - \hat{g}(\xi_k)|$, as a function of the number of splines is plotted in figure 6. For the 1s charge distribution, the error decreases with the number of splines and for the charge distribution of the shell, the error seems to oscillate but decrease overall.

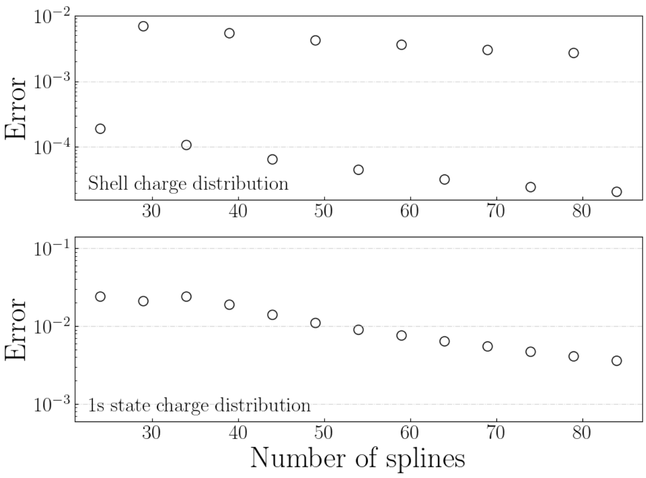

Figure 6: The maximum errors in the collocation points of the shell and hydrogen charge distributions when using the B-spline approximation.