# The electron-electron repulsion potential: programming module

*Develop*[*numerical procedure*](https://www.dsedu.org/courses/dft/veef)*to find e-e potential (Task 4) using Numerov (Task 5) and Thomas (Task 6) numerical methods.*

Our task is to find the electron-electron repulsion potential , if we know the radial wave function . For that we use Eq. (3) from [e-e potential](https://www.dsedu.org/courses/dft/tasks/vee), discretize it using finite differences to get the matrix equation (see [Numerov method](https://www.dsedu.org/courses/dft/tasks/numerov), Eq. (7)), and then solve the matrix equation by [Thomas method](https://www.dsedu.org/courses/dft/tasks/thomas).

Let us introduce new function



Our task is to solve numerically the following equation



where  is known radial wave function.

We will solve equation for , where points *ri* equally separate the range , here *r*0is a very small number and *rf* is sufficiently big number.

The boundary condition is



Since we use the finite region  we can write the boundary condition in the form



For  see Eqs. (5) and (6) from [e-e potential](https://www.dsedu.org/courses/dft/tasks/vee).

Then using [Thomas method](https://www.dsedu.org/courses/dft/tasks/thomas) we will look for solution in the form . For that, as a first step, we find coefficients  and  (see formula (4) in [Thomas method](https://www.dsedu.org/courses/dft/tasks/thomas)), and then, for second step, calculate the solution  using formula (3) from [Thomas method](https://www.dsedu.org/courses/dft/tasks/thomas).

For that using Eq. (4) for  we can define



Using Eqs. (4) from [Thomas method](https://www.dsedu.org/courses/dft/tasks/thomas) we can calculate ,  for .

For step two of [Thomas method](https://www.dsedu.org/courses/dft/tasks/thomas) (backward sweep) we calculate the functions . For that, using Eq. (4) we set  and then using recurrent formula (3) from [Thomas method](https://www.dsedu.org/courses/dft/tasks/thomas), we can calculate



for , whereas  is defined from Eq. (4).

The electron-electron repulsion potential then can be calculated using Eq. (1)

