# **Kohn-Shan equation solver: eigenvector**

*Develop*[*numerical procedure*](https://www.dsedu.org/courses/dft/ks_eigenvector)*to solve the radial KS equation with boundary conditions. Use Numerov and Thomas numerical algorithms.*

Here we consider how to find eigenvector of Kohn-Sham equation, if we know eigenvalue.

Let us write the radial Kohn-Sham equation for $1s$ state (see Eq. (4) from [Task 2](https://www.dsedu.org/courses/dft/tasks/ks)) in the form:



Eq. (1) can be solved by [Numerov method](https://www.dsedu.org/courses/dft/tasks/numerov).

We will solve equation on the region , where *r*0 is a very small number and *rf* is sufficiently big number. We separate this region evenly by points .

The boundary condition is



where  is the exact analytical solution considered in [Task 1](https://www.dsedu.org/courses/dft/tasks/h-atom) (see Eq. (6)).

Using [Thomas method](https://www.dsedu.org/courses/dft/tasks/thomas) we look for solution in the form  (see [Thomas method](https://www.dsedu.org/courses/dft/tasks/thomas), formula (3)). As a first step, we find coefficients  and  (see [Thomas method](https://www.dsedu.org/courses/dft/tasks/thomas), formula (4)), and for second step, calculate the solution .

Using Eq. for  we can define



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

For step two of [Thomas method](https://www.dsedu.org/courses/dft/tasks/thomas) we calculate the functions . For that, using Eq. 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. .