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

*Develop the*[*numerical procedure*](https://www.dsedu.org/courses/dft/ks_eigenvalue)*to calculate eigenvalue by integration KS equation.*

If we know the eigenvector , then the eigenvalue  can be calculated by integration of the radial Kohn-Sham equation (see [Task 4](https://www.dsedu.org/courses/dft/tasks/ks), formula (4)):



where  is the  Hamiltonian of the system, whereas  is the total KS potential. Then the eigenvalue can be calculated as



We calculate the integral in Eq. on the region . We suppose, that r0 is a sufficiently small number and rf is sufficiently big number so, that the integrals  and  can be neglected.