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# On the numerical solution of the two-centre Coulomb problem

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**Abstract**

An extensive literature is devoted to to investigating of the motion of an electron within the influence of two Coulomb centers with charges $Z_1$ and $Z_2$ located at a distance $R$ from each other (the so-called $Z_1eZ_2$ problem) [2]. Interest in this problem is constantly growing. At the same time, the computing apparatus used to determine the spectrum and the corresponding eigenfunctions is hopelessly outdated and does not allow massive calculations in a wide range of parameters.

It is known that the interaction potential of charges $Z_1$ and $Z_2$ with an electron allows separation of variables in the Schrödinger equation in spheroidal coordinates. However, in the bound-state problem ($E < 0$), complete separation is impossible, since the separated equations remain connected through a couple of spectral parameters - the energy of the state $E$ and the separation constant. Thus, a two-parameter spectral problem arises.

Previously, we have proposed efficient methods for solving two-parameter spectral problems arising from the separation of variables in spheroidal coordinates in the Helmholtz equation [1]. Despite the similarity of these problems, the application of the methods we have developed earlier is impossible without significant changes. The fact is that one of the boundary conditions imposed on the solutions of the radial equation obtained by separation of variables in the Schrödinger equation is square integrability over the entire positive semi–axis. The known asymptotic behavior of radial functions will allow us to transfer the integrability condition from infinity to a regular (finite) point. This means we replace the problem defined on the semi–axis with that one defined on a finite interval, while guaranteeing the preservation of the specified accuracy. The boundary condition at a regular point will depend on the current values of the spectral parameters, which will require some modification of our numerical methods.

The proposed numerical experiments will show agreement with previously known results, and the capability of the numerical method to handle various parameter choices.

**References**

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