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Numerical solution of elliptic boundary-value problems for Schrödinger-type equations using the Kantorovich method

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Abstract. Calculation schemes for numerical solution of elliptic boundary-value problems for Schrödinger-type equations based on Kantorovich method that reduces the initial problem to a set of boundary-value problems for a system of ordinary second-order differential equations are presented. The reduced boundary-value problems are discretized using the high-accuracy finite element method and implemented in the form of program complexes in Fortran 77. The efficiency of the calculation schemes and programs is demonstrated by the analysis of benchmark calculations of a boundary-value problem with 3D Schrödinger equation, describing the bound states in the nonrelativistic helium atom. Physical results of the symbolic-numeric analysis of low-dimensional quantum models using the developed method and software are discussed.

Keywords: elliptic boundary-value problems, Schrödinger-type equations, Kantorovich method, finite element method, helium atom, low-dimensional quantum systems

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