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POTHEA: a program for computing eigenvalues and eigenfunctions and their first derivatives with respect to the parameter of the parametric self-adjoined 2D elliptic partial differential equation. (English) Zbl 1360.35053

Comput. Phys. Commun. 185, No. 10, 2636-2654 (2014).

Summary: A FORTRAN 77 program is presented for calculating with the given accuracy eigenvalues, surface eigenfunctions and their first derivatives with respect to a parameter of the parametric self-adjoined 2D elliptic partial differential equation with the Dirichlet and/or Neumann type boundary conditions on a finite two-dimensional region. The program calculates also potential matrix elements that are integrals of the products of the surface eigenfunctions and/or the first derivatives of the surface eigenfunctions with respect to a parameter. Eigenvalues and matrix elements computed by the POTHEA program can be used for solving the bound state and multi-channel scattering problems for a system of coupled second order ordinary differential equations with the help of the KANTBP program [the second author et al., ibid. 177, No. 8, 649–675 (2007; Zbl 1196.81283)]. Benchmark calculations of eigenvalues and eigenfunctions of the ground and first excited states of a Helium atom in the framework of a coupled-channel hyperspherical adiabatic approach are presented. As a test desk, the program is applied to the calculation of the eigensolutions of a 2D boundary value problem, their first derivatives with respect to a parameter and potential matrix elements used in the benchmark calculations.

MSC:

35J25 Boundary value problems for second-order elliptic equations
65F15 Numerical computation of eigenvalues and eigenvectors of matrices
65L60 Finite element, Rayleigh-Ritz, Galerkin and collocation methods for ordinary differential equations

Keywords:

eigenvalue and multichannel scattering problems; Kantorovich method; finite element method; multichannel adiabatic approximation; ordinary differential equations; high-order accuracy approximations

Software:

ASYMPT; KANTBP; KANTBP 2.0; ODPEVP; POTHEA; POTHMF

Full Text: DOI

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