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Description of the FORTRAN program KANTBP 3.0 for computing energy levels, reflection and transmission matrices, and corresponding wave functions in the coupled-channel adiabatic approach

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Abstract. Description of the program KANTBP 3.0 implemented in FORTRAN for calculating energy values, reflection and transmission matrices, and corresponding wave functions in a coupled-channel approximation of the adiabatic approach is presented. In this approach, a multidimensional Schrödinger equation is reduced to a system of the coupled second-order ordinary differential equations (SOODEs) on a finite interval with the homogeneous boundary conditions of the third type at the left- and right-boundary points for continuous spectrum problem, or a set of first, second and third type boundary conditions for discrete spectrum problem. The resulting system of these equations containing the potential matrix elements and first-derivative coupling terms is solved using high-order accuracy approximations of the finite element method. Efficiency of the schemes proposed is demonstrated on an example of solution of quantum transmittance two-dimensional problem for a pair of coupled ions connected by the harmonic oscillator interaction through the repulsive Coulomb-like barriers. As a test desk, the program is applied to the calculation of the reflection and transmission matrices and corresponding wave functions of the boundary-value problem for a set of N coupled-channel SOODEs which follows from the above two-dimensional problem.

Keywords: Scattering and tunneling problems, coupled-channel adiabatic approach, reflection and transmission matrices, partial differential equations, finite-element method, high-order accuracy approximations

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