JMATRIX - Package for relativistic j-matrix calculations in elastic scattering of electrons from model potentials

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Abstrak

ABSTRAK
We present a software package JMATRIX1,consisting of two computer codes written in FORTRAN 95 and parallelized with OpenMP, implementing the so called J matrix method, applied to elastic scattering of electrons on the radial potential, vanishing faster than the Coulomb potential. In the J matrix method, the physical scattering problem is replaced by using a well defined model which is solved analytically. The presented software implements both non relativistic and relativistic versions of the method, and allows calculations of scattering phase shifts as well as cross sections, in cases when the scattering potential is given through an analytical formula. We performed test calculations for the scattering potential modeled as a truncated Coulomb potential. We show that the numerical phase shifts to converge as we increase the size of the basis used to truncate the scattering potential, and that the method is suitable for calculating the total diﬀerential momentum transfer and spin polarization cross sections, using the partial wave analysis.