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Numerical Aspects of Atomic Physics: Helium Basis Sets and Matrix Diagonalization ULRICH JENTSCHURA, JONATHAN NOBLE, Missouri Univ of Sci & Tech — We present a matrix diagonalization algorithm for complex symmetric matrices, which can be used in order to determine the resonance energies of auto-ionizing states of comparatively simple quantum many-body systems such as helium. The algorithm is based in multi-precision arithmetic and proceeds via a tridiagonalization of the complex symmetric (not necessarily Hermitian) input matrix using generalized Householder transformations. Example calculations involving so-called PT-symmetric quantum systems lead to reference values which pertain to the imaginary cubic perturbation (the imaginary cubic anharmonic oscillator). We then proceed to novel basis sets for the helium atom and present results for Bethe logarithms in hydrogen and helium, obtained using the enhanced numerical techniques. Some intricacies of "canned" algorithms such as those used in LAPACK will be discussed. Our algorithm, for complex symmetric matrices such as those describing cubic resonances after complex scaling, is faster than LAPACK's built-in routines, for specific classes of input matrices. It also offer flexibility in terms of the calculation of the so-called implicit shift, which is used in order to "pivot" the system toward the convergence to diagonal form. We conclude with a wider overview.

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