Accurate relativistic properties of hydrogenic atoms with the Lagrange-mesh method

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The Lagrange-mesh method is an approximate variational calculation using a special basis of N functions, called Lagrange functions, related to a set of N mesh points and the Gauss quadrature associated with this mesh [1]. It combines the high accuracy of a variational approximation and the simplicity of a calculation on a mesh [2,3]. The Lagrange functions are infinitely differentiable functions that vanish at all points of this mesh, except one. Used as a variational basis in a quantum-mechanical calculation, these functions lead to a simple algebraic system when matrix elements are calculated with the associated Gauss quadrature. The variational equations take the form of mesh equations with a diagonal representation of the potential only depending on values of this potential at the mesh points [1,3]. The most striking property of the Lagrange-mesh method is that, in spite of its simplicity, the obtained energies and wave functions can be as accurate with the Gauss quadrature approximation as in the original variational method with an exact calculation of the matrix elements [2,3]. It has been applied to various problems in atomic and nuclear physics.

For the exactly solvable Coulomb-Dirac problem describing hydrogenic atoms, numerically exact energies and wave functions, i.e. exact up to rounding errors, are obtained for any state and for any nuclear charge with very small numbers of mesh points [4]. Tests with the Yukawa potential provide very accurate results with a number of mesh points for which the computation seems instantaneous. The approximate wave functions provide mean values of powers of the coordinate that are also extremely precise. These results can be compared with very accurate benchmark calculations [5].

A more stringent test of wave functions is given by the calculation of polarizabilities. For the non relativistic hydrogen atom, numerically exact polarizabilities can be found with the Lagrange-mesh method for small numbers of mesh points [6]. Work is in progress to extend this study to the relativistic case, for which very accurate values are available for comparison [7]. In this case, exact static dipole polarizabilities are known only for the ground state [8] and the $2s$ excited state of the hydrogen atom [8,9]. Our aim is to calculate accurate numerical polarizabilities from the Dirac equation with the Lagrange-mesh method. We will use the obtained energies and wave functions from Ref. [4] to study multipolar polarizabilities of the ground state and some excited states in the hydrogenic and Yukawa cases.

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