Relativistic two-photon decay rates of hydrogenic atoms with the Lagrange-mesh method

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The simultaneous emission of two electric dipole photons is the dominant decay mechanism to the ground state for the $2s_{1/2}$ state of hydrogen [1]. This transition is one of the most widely studied atomic transitions in which selection rules forbid the emission of one electric dipole photon [2]. The calculation of this second-order process involves an infinite number of intermediate states. However, excellent results can be obtained with a finite number of pseudostates [1, 2, 3]. This calculation is simplified by the Lagrange-mesh method.

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 [4]. It combines the high accuracy of a variational approximation and the simplicity of a calculation on a mesh [5, 6]. 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 [4, 6].

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 [7]. Tests with the Yukawa potential also provide very accurate results. The approximate wave functions provide multipole polarizabilities that are also extremely precise [8].

In this work, we calculate accurate numerical two-photon decay rates from the Dirac equation with the Lagrange-mesh method. We use the obtained energies and wave functions from Ref. [7] to study the $2s_{1/2} - 1s_{1/2}$ transition in the hydrogenic and Yukawa cases. A test of the general requirement of gauge invariance for the relativistic results is successfully performed, which emphasizes the high accuracy of the numerical method for both types of potentials.

For a Coulomb potential, the results obtained for $Z = 1$ to 92 with the Lagrange-mesh method are in excellent agreement with a benchmark calculation involving Bernstein polynomial (B-polynomial) finite-basis sets [3]. For Yukawa potentials, we study the influence of the screening length on the $2s_{1/2}$ two-photon decay rate of a hydrogen atom embedded in a Debye plasma.

References

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