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COHERENT PROCESSES IN ATOM IN STRONG RADIATION FIELDS

February 1, 1991 - September 30, 1993

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During this grant period period work proceeded to study alternative methods of integrating the higher dimensional time-dependent partial differential equations that arise in the study of atoms interacting with intense laser radiation. Present methods use, for example, Taylor series propagators applied to finite-dfference and basis set models. We have more recently developed modified propagators based on polynomial extrapolation, rational polynomial extrapolation (Buelisch-Stoer), and have prepared versions that can be effectively vectorized on Cray YMP computers, and in the case of polynomial extrapolation, parallelize on massively parallel computers. In addition, the stability and accuracy of the finite-difference models has been compared to those based on interpolatory splines.

The main effort in this grant was directed toward developing numerical integrators for the Schroedinger equation describing the interaction on atoms with circularly polarized light. Previous work focused on the interaction of one- and two-electron atoms with linearly polarized light. In the case of one-electron atoms in linear polarized fields, the symmetry of the polarization axis could be exploited to reduce the 3-dimensional partial defferential equations to equations that are effectively 2-dimensional. With circularly polarized light, the full 3-dimensional equations must be solved. In the last year we have developed two successful approaches to the problem. The first approach is a basis set approach, in which the partial differential equations are written as large matrix equations on a basis of ortho-normal functions. This is an upgrade of the code used to integrate Schroedinger's equation in the linarly polarized case. The greater computational effort is evident in the increase requirements of CPU time in the 3-dimensional case. Problems that required 1.5 hours in the 2-dimensional case now require 30 hours on a Cray YMP. The method is appropriate for vectorizing super-computers, but does not yet run efficiently on massively parallel computers.

A finite-difference code for the 3-dimesional problem has been developed that runs efficiently on the CM-2 and CM-5 massively parallel computers. The method employs absorbing boundary conditions and the split-operator Richardson propagator. The absorbing boundary conditions are appropriate in studies of the the high harmonics of the laser radiation, which are calculated from the wave-function near the atomic core, far from the boundaries of the integration volume.

We have focused in the final stage on the theory of the interaction of one-electron atoms with intense, 2-color polarized laser radiation. Under these circumstances the atoms in intense fields emit high harmonics of circularly polarized radiation. (Monochromatic radiation will not generate harmonics.) We have now calculated the harmonic spectrum generated by one-electron atoms interacting with 2-color circularly polarized light of opposite helicities, and same helicities.

Publications:

Reports accepted for publication

"R-matrix theory of two-photon absorption: application to beryllium and carbon", M. W. Smith, K. T. Taylor, and C. W. Clark (**J. Phys. B: At. Mol. Opt. Phys.** in press).

Closed-form solutions of the Schroedinger equation for a model one-dimensional atom, W.-C. Liu and C. W. Clark (**J. Phys. B: At. Mol. Opt. Phys.** in press).

L. Pau, K.T. Taylor and C.W. Clark, *Convergence of Rayleigh-Schrodinger Perturbation Theory in Calculations of Multiphoton Processes*, Radiation Effects and Detects in Solids, 123, 725 (1991).

M.W. Smith, K.T. Taylor and C.W. Clark, *R-matrix theory of two-photon absorption: application to beryllium and carbon*, J. Phys. B: At. Mol. Opt. Phys., 25, 3985 (1992)

W.-C. Liu and C.W. Clark, *Closed-form solutions of the Schodinger equation for a model one-dimensional atom*, J. Phys. B: At. Mol. Opt. Phys., in press.

J. Parker and C.W. Clark, *Study of a plane-wave final-state theory for above-threshold ionization*, submitted to Phys. Rev. A.