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Relativistic dynamics for hydrogenlike systems

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Synopsis The interaction between super intense laser pulses and hydrogenlike systems is investigated. We aim to study cases where the field drives the electron up to velocities of $v \sim 0.5c$, where relativistic effects are believed to play a significant role. In order to investigate this, the time dependent Dirac equation (TDDE) has been solved numerically and comparisons are made to the predictions from solutions of the time dependent Schrödinger equation (TDSE).

The strong development in laser technology has lead to pulses with increasing intensities and higher photon energy. Given the extreme peak intensity expected in the future, for instance at the X-ray free electron laser facilities, it is of great importance to explore the role of relativistic effects in light-matter interaction predicted by the TDDE.

Doing so however poses quite some challenges. First, the spectrum of the time independent Dirac equation contains negative energy states (NES). Since these are connected to the description of positrons one might expect that they can be neglected as long as the field strength is far below the limit for electron-positron pair-production. This is however, in general, not the case since the NES are required to even get the correct non-relativistic limit [1, 2]. Together with the spin degree of freedom the NES make the basis set within each symmetry four times larger than in the non-relativistic case. Second, not only is the computational load heavy due to a larger basis set within each symmetry but the total number of symmetries required for convergence in a simulation seems to increase when the NES are included. Finally, for field strengths where a relativistic treatment is called for one also expects effects beyond the dipole approximation to be important. This increases the number of couplings significantly since the electron can now change m-quantum numbers even with linearly polarized light.

Here we will present various results obtained from a numerical solution of the full-dimensional TDDE beyond the dipole approximation. The spatial part of the vector field is represented through a power series expansion up to fourth order and the convergence of this expansion at different field strengths will be compared.

To handle the computational demand we employ complex scaling to minimize the basis set and a second order Magnus propagator for time propagation. The propagation is significantly speeded up by the use of a Krylov subspace technique and parallelized routines for matrix operations.

Figure 1 shows the ionization yield of hydrogen with the electron initially prepared in the ground state, exposed to a pulse of the form $\mathbf{A}(\omega t - kx) = \frac{E_0}{\omega}\sin^2\left(\frac{\omega t - kx}{2N}\right)\sin(\omega t - kx)\,\hat{\mathbf{e}}_z$. In this example the number of optical cycles is $N = 10$, the central frequency is $\omega = 3.5$ a.u. and the peak electric field strength E_0 is varied.

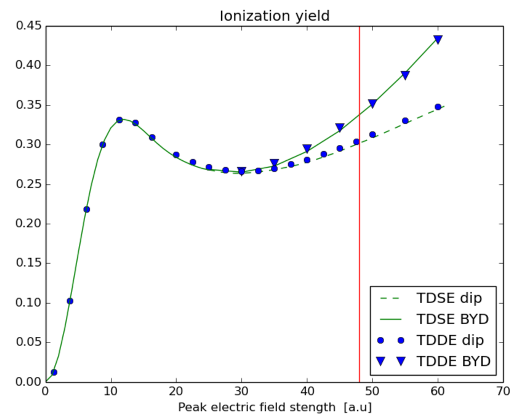

Figure 1. Ionization yield of hydrogen for the electron initially prepared in the ground state. The acronym BYD stands for beyond dipole approximation. The vertical line denotes the field strength where the electron obtains a velocity $v \sim 0.1c$.

References

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