Effects of numerical approximations in the treatment of short-pulse strong-field ionization of atomic hydrogen

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We solve the time-dependent Schrödinger equation for the hydrogen atom exposed to strong-field few-cycle laser pulses with the central photon energy corresponding to the $1s \rightarrow 2p$ transition. Comparison with results from other recent calculations suggests that the approximations made in those works produced inaccuracies that shed doubt on the physical effects predicted at large photoelectron energies.

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As the only neutral atomic target, for which the nonrelativistic wave functions are known exactly, atomic hydrogen remains the ideal system to study fundamental processes such as its interaction with an external electromagnetic field. Instead of attempting a comprehensive list of references, we illustrate this interest by listing a few papers that appeared within the past few months in this journal [1–4]. Atomic hydrogen is also an excellent system to investigate a variety of models and numerical methods, especially the validity of approximations that may be required for more complex systems, since it is now possible to generate theoretical benchmark results with a high degree of confidence. In fact, combining accurate theoretical with experimental data in the hydrogen atom was recently used to determine the absolute intensity of a laser to unprecedented accuracy at the 1% level [5].

One of the approximate methods mentioned above was recently introduced by Nganso *et al.* [6]. The basic idea is to replace the kernel of the nonlocal Coulomb potential in the momentum-space representation of the problem by a finite sum of separable potentials. This allows for the three-dimensional time-dependent Schrödinger equation (TDSE) to be reduced to a system of coupled one-dimensional linear Volterra integral equations, the numerical solution of which is relatively easy to obtain.

In the calculations of [6], the separable potentials supported only the hydrogen $1s$, $2s$, and $2p$ discrete states. The accuracy of the method was then tested by comparison against predictions from a numerical solution of the TDSE, based on a Sturmian expansion described by Madroñero and Piraux [7]. The comparison (see Fig. 8 of [6]) was assessed as "qualitatively correct." The strength of this assessment, however, should be viewed in the context that Madroñero and Piraux themselves showed cases where some of their results were apparently not converged. These cases were later discussed in some detail by Grum-Grzhimailo *et al.* [8], who adopted the matrix-iteration approach of Nurhuda and Faisal [9]. In the meantime, results from the latter approach were compared on several occasions against those from an entirely independent Arnoldi-Lanczos time-propagation scheme developed by Ivanov and Kheifets (see, for example, Ref. [10]), always yielding excellent agreement between the predictions from these two methods. Consequently, we believe that our approach is sufficiently stable to truly test the predictions of approximate algorithms such as that put forward by Nganso *et al.* [6].

Apart from the comparison with the results from the Sturmian approach in Fig. 8 of [6], Fig. 4 of the above paper also contains some surprising results regarding the underlying physics. Specifically, the Autler-Townes doublet structure [11] in the ejected electron energy distribution function is flattening out for electron energies above approximately two atomic units (a.u.). For the (central) photon energy of 0.375 a.u. and a comparatively low peak intensity of 4×10^{14} W/cm^2, however, such a plateau would generally not be expected. Hence, the question arises whether this prediction is possibly indicating some "new physics," maybe related to the fact that this energy corresponds to the $1s \rightarrow 2p$ resonance transition, or whether it is simply an artifact of the model and/or of the numerical approximation. To our knowledge, the photoelectron spectra obtained by direct numerical solving of the TDSE under the resonance conditions ($\omega = 0.375$ a.u.) have been presented in the literature only for electron energies up to 1.5 a.u., i.e., including just the lowest three above-threshold ionization (ATI) peaks [12–16].

The principal purpose of the work presented in this report is to validate the model of Nganso *et al.* [6] once again, namely against the results from solving the TDSE directly on a numerical grid. In particular, we are interested in the existence, or lack thereof, of the predicted plateau structure at high ejected electron energies.

Our numerical method was described in detail by Grum-Grzhimailo *et al.* [8]. Briefly, we use the matrix iteration method MIM of Faisal and Nurhuda [9] to propagate the initial field-free state (atomic hydrogen with its electron in the $1s$ ground state) in time under the influence of a strong laser pulse. Depending on the peak intensity of the pulse, we use either the length or the velocity form of the electric dipole operator. We check that the results from the two formulations agree within the thickness of the line when the form of the

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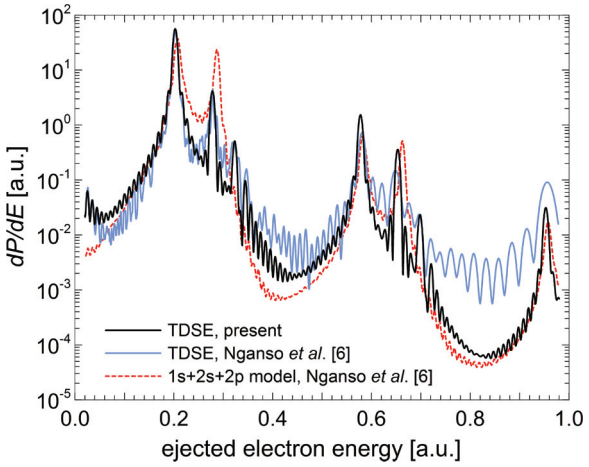

FIG. 1. (Color online) Ejected electron spectrum for a 40-cycle laser pulse with central photon energy of 0.375 a.u. and a peak intensity of $4.0 \times 10^{14}\mathrm{W/cm}^2$. The envelope function for the electric field is of trapezoidal form, ramping on and off over two optical cycles with a plateau of 36 cycles. Results from our numerical solution of the TDSE are compared with those presented by Nganso *et al.* [6].

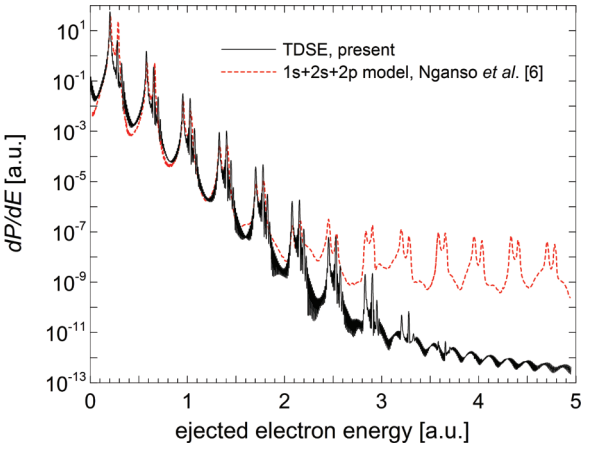

FIG. 2. (Color online) Same as Fig. 1, except for an extended range of ejected electron energies and without TDSE results from the Sturmian approach.

operator is switched from one to the other for cases where both forms are numerically suitable.

Furthermore, we ensure that the final predictions are, once again within the thickness of the lines in the figures, independent of the number of partial waves used in the expansion of the wave function. And, finally, we performed several spot checks to verify that the results are independent of the numerical parameters such as the grid spacing, the time step, the radius of the absorbing gobbler, and the number of iterations.

Figures 1 and 2 exhibit the ejected electron spectrum for a 40-cycle laser pulse with central photon energy of 0.375 a.u., corresponding to the $1s \rightarrow 2p$ resonance transition. The peak intensity is 4.0×10^{14} W/cm^2 (peak electric field 0.10676 a.u.), and the envelope function for the electric field is of trapezoidal form, ramping on and off over two optical cycles with a plateau of 36 cycles. The identical pulse was used by Nganso *et al.* [6].

Figure 1 exhibits results for ejected electron energies up to 1 a.u. We note a much better agreement between the predictions from our solution of the TDSE and the approximate results of Nganso *et al.* [6] than what the latter authors found in their comparison with the results from the Sturmian expansion in the solution of the TDSE.

The main photoelectron line and the first ATI line, as obtained in our numerical solution of the TDSE, exhibit fine structure that was already studied in some detail earlier. In particular, the first two peaks at the electron energies of about 0.20 a.u. and 0.28 a.u. correspond to the Autler-Townes doublet, which originates from ionization of the $2p$ state resonantly coupled to the $1s$ state. A few more clearly distinguishable peaks on the high-energy shoulder of the main photoelectron line, albeit with decreasing intensity, are due to ionization of the $3p$ and $4p$ intermediate states that are transiently populated during the pulse. Peaks due to ionization from even higher-lying np states effectively vanish in the background [13,15]. Our TDSE calculations predict smaller widths of the Autler-Townes components in comparison with the model of [6] and a smaller relative intensity of the high-energy component. In accordance with the Floquet analysis of Girju *et al.* [14] and the predictions of Nganso *et al.* [6], the left subpeak is broader than the right one due to the higher ionization rate of the lower dressed state.

Figure 2 shows the ejected-electron spectrum over an extended range of ejected electron energies. As mentioned above, Nganso *et al.* [6] predict a plateaulike energy dependence for ejected electron energies above approximately 2 a.u. This is surprising in light of the expected small ponderomotive potential for this case. Indeed, this predicted energy dependence is *not* confirmed by our solution of the TDSE and appears to be an artifact of the model. It would be interesting to add separable potentials that support hydrogen states with $n > 2$ in the approach of [6], in order to see whether the predicted plateau effect remains. We believe that our approach, ultimately, also encounters numerical challenges that prevent us from obtaining accurate numbers that are 11–12 orders of magnitude smaller than the peak values.

To summarize, we carried out calculations to describe the interaction of a short strong laser pulse with the hydrogen atom. Using a well-tested computer code, we compared the predictions with those from previous numerical calculations. Our results are in agreement with general expectations regarding, for example, the lack of a substantial plateau in the ejected electron spectra for photon energies in the VUV range and relatively low peak intensities.

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