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Dynamics of a one-dimensional model and a three-dimensional hydrogen atom in an intense high-frequency short-pulse laser

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We present nonperturbative calculations of ionizing and trapping probabilities for a one-dimensional model and a three-dimensional hydrogen atom in an intense high-frequency Gaussian-pulsed laser field. Investigating the dynamics of the ionization process (for one- and two-photon ionization), we find that only for extremely short pulses, especially for hydrogen, does the system have a significant probability of surviving at the end of the pulse, leading to the phenomenon of atomic stabilization with respect to ionization. We also find that a one-dimensional model has a higher survival probability at the end of a Gaussian pulse, as compared to the three-dimensional hydrogen atom.

The behavior of an atom under a superstrong, high-frequency field has been attracting quite a bit of attention in the community of theoretical multiphoton physics. This pertains to the question of possible stabilization with respect to ionization under such conditions as proposed by Pont *et al.* [1,2]. A more recent paper by Pont and Gavrila [3] has raised considerable doubt about the possible direct experimental observation of such an effect. Having now evaluated the possibility for the atom to survive the lower (in relative terms) intensities during the rising and falling of the pulse, these authors obtain a negative answer. As has been shown in Ref. [4], the explicit time dependence of the laser intensity due to its pulsed nature plays a fundamental role in understanding the processes of interaction with strong fields and unless it is included in a calculation, one cannot be sure about the validity of the prediction. The calculation of Pont and Gavrila [3] on the other hand, being inherently time independent, provides only average lifetimes at fixed intensities and not the complete time evolution of the system in a realistic pulse.

There would be no doubt about the theoretical prediction of atomic stabilization with respect to ionization, if an atom could be exposed to a constant superstrong and high-frequency field. This has been proved by both time-independent [1,2,5] and time-dependent [6,7] calculation. Since high power lasers are inevitably pulsed, one of the major questions has to do with the dynamics of an atom in such a *realistic* laser *pulse*. The answer has been complicated further by the results of one-dimensional atomic models, which are easier to handle computationally but lack many of the fundamental properties of a real atom.

In this paper, we present results of one- and three-dimensional quantum-mechanical calculations for a hydrogen atom in an intense *pulsed* laser field. We use a pulse consisting of a Gaussian shape of the field which will obviously expose the atom to intensities lower than the peak one not only during the rise but also during the fall of the pulse.

The calculations reported here were performed in terms of square-integrable basis sets, [8] and in the framework of nonrelativistic quantum mechanics and in the dipole approximation as has been the case with all related calculations. The time-dependent wave function of the electron is obviously going to spread out as a function of time. In this sense the length gauge form of the dipole interaction (the E gauge), which is proportional to $\mathbf{r}$, will increase without bound, and, as pointed out by Kulander, Schafer, and Krause [7] recently, it will require much more effort to achieve numerical convergence in the results. Therefore we first convert the Hamiltonian to the velocity gauge form of the dipole interaction (the A gauge). As the A^2 term can be adsorbed in a phase factor which does not affect the populations, the Schrödinger equation for the correctly transformed effective wave function is

$$i\hbar\frac{\partial}{\partial t}\Psi_A(\mathbf{r},t)=[H^0+e\mathbf{A}(t)\cdot\mathbf{p}/mc]\Psi_A(\mathbf{r},t)\,. \quad (1)$$

Here H^0 is the Hamiltonian of the unperturbed atom and the vector potential $\mathbf{A}(t)$ is related to the electric field $\mathbf{E}(t)$ by $\mathbf{E}(t)=-(1/c)(\partial/\partial t)\mathbf{A}(t)$. Due to the assumed Gaussian pulse shape, the asymptotic values for both the field and the vector potential are $\mathbf{E}(\pm\infty)=\mathbf{0}$ and $\mathbf{A}(\pm\infty)=\mathbf{0}$. The relation between the wave function Ψ_E in the E gauge and the wave function Ψ_A in the A gauge is given by the well-known Göppert-Mayer transformation:

$$\Psi_E(\mathbf{r},t)=e^{ie\mathbf{r}\cdot\mathbf{A}(t)/\hbar c}\Psi_A(\mathbf{r},t)\,. \quad (2)$$

To obtain the final results in the E gauge, in principle one should first convert the initial-state wave function of H^0 to the A gauge, perform the time integration, and then convert the solution back to the E gauge before calculating the population or probabilities [8]. The use of a Gaussian pulse shape will make the gauge transformation not necessary, since we will be interested only in the wave function at the end of the pulse.

We choose the vector potential to have the form

$$\mathbf{A}(t)=\boldsymbol{\epsilon}\frac{cE_0}{\omega}\cos(\omega t)f\left(\frac{t}{\tau}\right), \tag{3}$$

where $\boldsymbol{\epsilon}$ is the unit polarization vector and $f(t/\tau)$ has the form $e^{-(t/\tau)^2/2}$. More details about the method of calculations can be found elsewhere [8].

As a test for the method and the invariance under the gauge transformation, we first calculate single-photon ionization of hydrogen at different peak intensities (which defined as $I_0=cE_0^2/8\pi$, is considered more as a parameter of the numerical calculation than a quantity with a physical counterpart, since a rigorous definition of intensity for very short pulses is impossible), by using both the length and the velocity gauges. Because of the short pulse duration, the time derivative of the pulse envelope function f cannot be neglected in the definition of electric field in terms of the vector potential. With the above definition of the vector potential, the electric field is then

$$\mathbf{E}(t)=\boldsymbol{\epsilon}E_0\left[\sin(\omega t)+\frac{t}{\omega\tau^2}\cos(\omega t)\right]f\left(\frac{t}{\tau}\right). \tag{4}$$

The results listed in Table I show a perfect agreement (when attention is paid to the correct definition of the electric field) between the length and the velocity forms of the interaction for the populations of the ground state and the total population in the continuum (positive energy) states, at the end of the pulse with $\tau=5$ optical cycles. Through this test, we also found that increasing the peak intensity to higher and higher values, we have increasingly greater difficulty in obtaining numerically converged results when using the length gauge. This is because not only in the length gauge more CPU time is needed to perform the time integration (even with the same number of basis functions in both gauges), but also the length gauge requires more angular momentum functions to get the same degree of accuracy with respect to the velocity gauge. This result is consistent with the conclusion drawn in Ref. [7].

We have also numerically tested (for the sake of brevity the results are not presented here) that the relative importance of the second term in the definition of the electric field in Eq. (4) actually decreases with increasing the value of τ. Obviously, for $\tau \gg 2\pi/\omega$, a correct definition of the intensity in terms of the time average of the square of the electric field over one optical cycle becomes possible.

After having gained some confidence in the gauge invariance of our results, we have performed numerical calculations for both the very popular one-dimensional model (the so-called soft-core model) and the real hydrogen atom. We have investigated the surviving probability at the end of the pulse in a range of intensities for which the ionization rate is believed to be strongly suppressed. The binding potential [6] for this one-dimensional model is

$$V(x)=-\frac{1}{(1+x^2)^{1/2}}. \tag{5}$$

The ionizing threshold for this model potential is 0.6698 a.u. The behavior of this one-dimensional model under a strong radiation field has been extensively investigated [6,9,10]. The stabilization of this model against ionization in intense, high-frequency radiation fields has been recently related to the properties of the x-p phase space [11].

While there is no doubt about the usefulness of one-dimensional calculations in very specific systems (e.g., solid-state systems), their reliability in obtaining useful physical information for intrinsically three-dimensional problems (like the general field of laser-atom interactions) is highly questionable. The conclusions, derived from the analysis of such a simplified one-dimensional model, concerning the requirements upon intensity and frequency for the stabilization of real atoms in *superintense* laser fields, have been recently questioned on the basis of a purely classical analysis [12].

Using a general nonperturbative method which was developed and presented most recently [8], we are in the position to obtain answers to this question for a one-dimensional model as well the real three-dimensional

TABLE I. Comparison between length and velocity gauge results for the populations of the ground state (g) and of the continuum states (c) at the end of the pulse with $\tau=31.4159$ a.u. (5 optical cycles) for three-dimensional hydrogen with photon energy $\hbar\omega=1$ a.u. The peak intensity I_0 is expressed in terms of the atomic unit $I_a=3.51\times10^{16}$ W/cm^2.

Intensity I_0 (a.u.)	Length gauge g	Length gauge c	Velocity gauge g	Velocity gauge c
0.005	0.9507	0.0493	0.9507	0.0493
0.025	0.7773	0.2227	0.7772	0.2228

TABLE II. The populations of ground and continuum states at the end of the pulse for the one-dimensional soft-core model of hydrogen with $\hbar\omega=1$ a.u. The velocity gauge has been used. Symbol definition as in Table I.

Intensity I_0 (a.u.)	$\tau=50$ a.u. g	$\tau=50$ a.u. c	$\tau=100$ a.u. g	$\tau=100$ a.u. c	$\tau=150$ a.u. g	$\tau=150$ a.u. c
1	0.0574	0.9426	0.0033	0.9967	0.0002	0.9981
5	0.0293	0.9707	0.0008	0.9992	0.0000	0.9999
10	0.0686	0.9314	0.0046	0.9954	0.0008	0.9992
25	0.1039	0.8960	0.0103	0.9897	0.0006	0.9994
50	0.1283	0.8712	0.0164	0.9836	0.0028	0.9972
100	0.1356	0.8365	0.0245	0.9755	0.0039	0.9960

TABLE III. The populations of ground and continuum states at the end of the pulse for the one-dimensional model of hydrogen with $\hbar\omega=0.44522$ a.u. (two-photon ionization at low field). The velocity gauge has been used. Symbol definition as in Table I.

Intensity I_0 (W/cm^2)	$\tau=50$ a.u. g	$\tau=50$ a.u. c	$\tau=100$ a.u. g	$\tau=100$ a.u. c	$\tau=150$ a.u. g	$\tau=150$ a.u. c
2×10^{16}	0.0856	0.8482	0.0048	0.9860	0.0002	0.9992
5×10^{16}	0.0428	0.8461	0.0086	0.9761	0.0006	0.9994
10^{17}	0.0672	0.7373	0.0155	0.9647	0.0017	0.9942
2×10^{17}	0.1072	0.7440	0.0244	0.9395	0.0025	0.9933

TABLE IV. The populations of ground and continuum states at the end of the pulse for three-dimensional hydrogen with $\hbar\omega=1$ a.u. The velocity gauge has been used. Symbol definition as in Table I.

Intensity I_0 (a.u.)	$\tau=12.56637$ a.u.		$\tau=31.4159$ a.u.		$\tau=62.8318$ a.u.	
	g	c	g	c	g	c
0.2	0.453	0.547	0.140	0.861		
1	0.037	0.963	0.001	0.999		
5	0.034	0.962	0.001	0.999		
25	0.054	0.872	0.001	0.998	0.000	1.000
50	0.043	0.823	0.004	0.992	0.000	1.000
100	0.028	0.755	0.006	0.976	0.000	1.000

atom, even if more than one electron is involved. Our purpose in this paper is to focus upon a precise evaluation of the difference between the one-dimensional model and the real three-dimensional atom, and to demonstrate the importance of the pulsed nature of the field.

In Table II we show numerical results for the ground and continuum state populations at the end of the pulse for the one-dimensional model described above. The photon energy is such that the parameter $\alpha_0=I_0^{1/2}/\omega^2$ a.u. ranges from 1 to 10. The intensity dependence of the continuum states' population shows a maximum which is particularly evident for the smallest value (50 a.u. ≈ 8 optical cycles) of the pulse-shape parameter τ. The presence of this maximum is hardly seen for values of τ larger than 16 optical cycles.

The same general behavior can be seen in Table III. The photon energy is now such as to require a two-photon ionization at low fields and the parameter α_0 is in the range from 1.7 to 5.36.

In Table IV we show numerical results for three-dimensional hydrogen. The parameter α_0 ranges from 0.45 to 10. We can see that a very small value of τ (in the first column τ is equal to 2 optical cycles which is almost four times smaller than the smallest one used in the one-dimensional model) is required to show significant evidence of the suppression of the ionization. We can also see from Table IV that even with a pulse parameter τ as short as 5 optical cycles ($\tau=31.4159$ a.u. $=0.76$ fs), which is of course unrealistic, any significant suppression of the ionization at the end of the pulse is hardly seen. This is in agreement with the analysis of Ref. [12], stating that the requirements of high intensity and high frequency are less strict for one-dimensional than for real three-dimensional systems.

We would like to point out that in our calculations 90% or more of the ionization takes place during the rise of the pulse, at least at high values of the peak intensity, while the pulse consists of a symmetric rising and falling shape. This asymmetry of the ionization under a symmetric pulse is due to the fact that, initially, the atom is in the ground state which is the orbital closest to the nucleus and has the largest chance to absorb protons, while after passing the peak value of the intensity, almost everything is in excited states which have less chance to absorb photons, since they have a smaller probability to get close to the nucleus. More detailed results on ionization from excited states will be discussed in a future paper [13].

We undertook this investigation with a dual purpose. First we wanted to explore the possible danger in drawing conclusions about the dynamics of atoms in strong fields on the basis of one-dimensional models. Our results have indeed demonstrated that under realistic pulse conditions the one-dimensional model produces stabilization that cannot be expected from the real atom.

Second, we wanted to produce realistic results for the real three-dimensional hydrogen atom under realistic pulse shapes. Choosing a frequency sufficiently high and a range of intensities beyond present day possibilities (for that frequency) we have shown that suppression of ionization (in the sense of decreasing ionization with increasing intensity) is obtained only for unrealistically short pulses ($\tau\approx 0.3$ fs). The effect disappears for slightly longer, but sill unrealistically short ($\tau\approx 0.76$ fs) pulses. The effect found for the shorter pulses can be understood as a consequence of populating excited states—owing to the enormous bandwidth of the pulse (Fourier width)—which do not ionize easily during the time available to them. It should be noted that this aspect of the phenomenon is not (cannot be) included in the predictions of time-independent calculations. We can also seen from Table IV that probabilities for trapping into higher exited states are quite dramatic for $\tau\approx 0.3$ fs and $\alpha_0\geq 5$ at end of the pulse, but that the trapping probabilities are decreasing as τ increases, which, of course, connected to suppression of ionization and can be also understood as an effect of the Fourier bandwidth.

We could continue with calculations at higher frequencies and intensities. We believe, however, that they would be nothing more than mathematical exercises, since our present combination of frequency and intensities already extends well beyond realistic expectations for the foreseeable future.

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