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Ionization of the hydrogen atom: from weak to strong static electric fields

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Abstract. We present a study of the ionization of the hydrogen atom by weak and strong static electric fields from the ground state and from some excited states. The under- and above-ionization barrier dynamical regimes are accurately computed for short and long times. The results are interpreted through the spectral density which emphasizes, for transitory regimes, the role of the resonances arising from the ground and from the lowest excited states. The observability of the dynamics is discussed.

PACS. 32.60.+i Zeeman and Stark effects – 32.70.Cs Oscillator strengths, lifetimes, transition moments – 32.70.Jz Line shapes, widths, and shifts

1 Introduction

The decay of the ground state of the hydrogen atom exposed to a static electric field has been the subject of many studies since the beginning of quantum mechanics. Most of the investigations have been done at low fields. The ground state is an isolated resonance and the atom ionizes by tunneling effect. In this domain, the quasi-classical theory provides a satisfactory simple expression of the ionization rate [1]. At higher fields ionization proceeds directly above the Coulombic barrier created by the external field. Up to now only a limited work has been done at high field, generally restricted to short-time dynamics [2,3]. Geltman wrote in [3]: "... A complete treatment by Stark broadening theory that would be applicable to all t has not yet been carried out...". Since at short times the dynamics of the ionization from the ground state implies the lowest excited states, we have also investigated the dynamics of the ionization starting from the excited states $2s$ and $2p$. Although the whole ionization process is irreversible transitory oscillating regimes may appear. It is noteworthy that the hydrogen atom which possesses only one electron may generate a large range of reversible and irreversible processes. Therefore it is justified to perform an overall study of the various decay regimes in weak, intermediate and strong fields. We will focus on the various time scales relevant to the dynamics. A special emphasis will be given to non-expotential decays which do not seem to have been studied previously, especially within the tunneling regime.

It is important, for computing and understanding the dynamics, to master the mean lifetimes of the ground state and of the lowest excited states implied in the ionization process [3]. The excited states are more polarizable than the ground state and their lifetimes are much shorter than the lifetime of the ground state. It results that computing accurately the dynamics of the ionization at short times and at long times requires an accurate determination of the various characteristic time scales. In close-coupling approaches much attention must be paid for avoiding spurious reflections arising from the use of finite grids or of a finite number of basis functions [3,4]. Consequently some smoothing, or filtering or averaging procedure is needed for determining the Green's functions (spectral densities) which provide the relevant widths. Many techniques are available for performing analytical continuation, the most current being to add an optical potential [5] (or a complex absorbing potential [6]) to the Hamiltonian or to complex-rotate the dissociative electronic variable in the Hamiltonian [7]. It has been shown that complex scaling and the use of a simple basis of Slater orbitals lead to accurate widths of the resonances arising from the $1s$, $2s$ and $2p$ states [8,9]. Complex scaling provides also an accurate description of the depletion of the ground state for the intermediate value of the electric field $\mathcal{E} = 0.08$ a.u. [2,4]. Therefore we have chosen to apply this method for computing, describing and interpreting the results. The Green's functions yield the relevant energies, widths and oscillator strengths. The survival and

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transition probabilities are immediately obtained by the inverse Laplace transformation. The theory will be briefly recalled in Section 2. The dynamics of the ionization from the ground state will be investigated in Section 3. Various ionization processes arising from the state $2s$ and $2p$ will be presented in Section 4.

2 Theory

A constant electric field of amplitude $\mathcal{E}$ is applied to the hydrogen atom. At the initial time $t = 0$ it is assumed that the atom is in the ground state. The time-dependent wave function proceeds as

$$|\psi(t)\rangle = \mathrm{e}^{-\mathrm{i}\,Ht/\hbar}|1s\rangle; \qquad (t > 0). \tag{1}$$

As soon as the atom is exposed to the field, the ground state becomes a resonance and the atom begins to ionize. Since we aim to study the dynamics of the ionization process we shall determine the probability of remaining in the initial state (survival probability) at the time t:

$$P(t) = |\langle 1s|\psi(t)\rangle|^2. \tag{2}$$

A deeper insight into the dynamics is obtained by an energy analysis of the initial state given by the lineshape (spectral density) [10]

$$I(E) = -\frac{1}{\pi}\mathrm{Im}\, G(E). \tag{3}$$

$G(E)$ is the Green's function associated with the ground state. By extending the variable energy E in the complex plane (variable z), the Green's function is expressed as

$$G(z) = \langle 1s|\frac{1}{z-H}|1s\rangle. \tag{4}$$

The survival probability amplitude is the inverse Laplace-Fourier transform of the Green's function:

$$\langle 1s|\psi(t)\rangle = \frac{1}{2\pi\,\mathrm{i}}\int\limits_C G(z)\,\mathrm{e}^{-\mathrm{i}\,zt/\hbar}\mathrm{d}z \qquad (t > 0). \tag{5}$$

In (5) the integration path C runs on the real energy axis from $+\infty$ to $-\infty$ and is closed in the lower part ($\mathrm{Im}\, z < 0$) of the complex plane. Since there is no elementary way to solve the problem analytically we will determine numerical solutions. We consider the usual Hermitian Hamiltonian in Cartesian coordinates:

$$H = -\frac{\Delta}{2} - \frac{1}{r} - \mathcal{E}z. \tag{6}$$

By complex-rotating the coordinates [7], the Hamiltonian (6) becomes

$$H_\theta = -\frac{\Delta}{2}\mathrm{e}^{-2\mathrm{i}\theta} - \frac{1}{r}\mathrm{e}^{-\mathrm{i}\theta} - \mathcal{E}z\mathrm{e}^{\mathrm{i}\theta}. \tag{7}$$

θ is the angle of rotation. From (6) and throughout this paper we will use atomic units (a.u.). The diagonalization of the Hamiltonian (7) in a finite basis set of N square-integrable functions provides a finite number of eigensolutions $\mathcal{E}_k$, $|\psi_k\rangle\,(k = 1, 2, ...N)$. Then the Green's function (4) may be written as

$$G(z) = \sum_k \frac{f_k}{z - \mathcal{E}_k}. \tag{8}$$

The f_k's are generalized oscillator strengths [10]:

$$f_k = \langle 1s|S^{-1}|\psi_k\rangle(\psi_k|S|1s\rangle; \quad S = \mathrm{e}^{\mathrm{i}\theta r\frac{\mathrm{d}}{\mathrm{d}r}}; \quad \sum_k f_k = 1. \tag{9}$$

The oscillator strengths play an important role for discussing the lineshapes (3) and the various dynamical regimes. Using (8) the survival amplitude (5) may be expressed as

$$\langle 1s|\psi(t)\rangle = \sum_k f_k \mathrm{e}^{-\mathrm{i}\,\mathcal{E}_k t/\hbar}. \tag{10}$$

Ionization from excited states proceeds along the same lines as for the ground state. If we assume that the atom is in the state $|i\rangle$ at the initial time, expressions (1) to (9) remain valid by replacing $|1s\rangle$ by $|i\rangle$. The dynamical information for computing the transition probabilities between two states requires the determination of the Green's function:

$$G_{ij}(z) = \langle i|\frac{1}{z-H}|j\rangle = \sum_k \frac{f_{ij,k}}{z - \mathcal{E}_k}, \tag{11}$$

where

$$f_{ij,k} = \langle i|S^{-1}|\psi_k\rangle(\psi_k|S|j\rangle; \quad \sum_k f_{ij,k} = \delta_{ij}. \tag{12}$$

It is assumed in (11) and (12) that the states $|i\rangle$ are orthonormal.

The numerical calculations were done by using a finite basis set of 320 Slater orbitals of the form

$$\varphi_{l,k} \propto r^{k-l-1}\mathrm{e}^{-\zeta\, r}\, Y_{l,0}\,(\theta, \phi); \quad k = l + 1, 2...l + 40. \tag{13}$$

The orbital quantum number runs from $l = 0$ to $l = 7$ and $\zeta = 1$. The orbitals were symmetrically orthogonalized and we have kept $N = 175$ numerically linearly independent functions. Finally, the summation over k, in (8) and (9), is limited to $M < N$ values of k corresponding to the eigenenergies having negative imaginary parts ($\simeq$ outgoing boundary conditions). The values of M were found to be near $N = 175$, for example, $M = 169$ for $\mathcal{E} = 0.005$ a.u. and $M = 130$ for $\mathcal{E} = 1$ a.u. For any value of the electric field the closure relation over the oscillator strengths is accurately satisfied. The greatest discrepancy $1 - \sum_k f_k = 0.000019 + \mathrm{i}\,0.000029$ occurs for the highest value of the electric field $\mathcal{E} = 1$ a.u. We have carefully checked that the observable quantities (lineshapes and survival probabilities) did not depend in a large extend on the parameters of the basis: the exponent ζ, the number of angular symmetries l and the number of orbitals for each value of l. In addition, we have verified that the results did not depend on the angle of rotation θ within the interval [0.2–0.4]. We have also compared our results for $\mathcal{E} = 0.08$ a.u. with the dynamics found by Scrinzi [2] (see Sect. 3.2).

3 Ionization from the ground state

The frontier between weak and strong coupling appears for $\mathcal{E} = 0.0625$ a.u. when the energy of the ground state becomes equal to the energy at the top of the potential barrier generated by the electric field. For fields $\mathcal{E} \leq 0.02$ a.u. the coupling with the continuum is weak and the isolated Weisskopf-Wigner resonance has an almost exponential decay. This weak coupling regime was fully investigated for many years by many methods. However, it still remains to investigate the transitory regimes at short times. For strong electric fields, $\mathcal{E} \gg 0.1$ a.u., a complete treatment of the problem has not yet been done. Let us now study the evolution of the dynamics of the ionization for the weak, intermediate and strong couplings.

3.1 Weak coupling ($\mathcal{E} \leq 0.02$ a.u.)

The ground state 1s is an almost pure Weisskopf-Wigner resonance weakly coupled to the continuum. The width of the resonance and the survival probability are approximatively given by the quasi-classical theory [1]:

$$\Gamma(\text{a.u.}) = \frac{4}{\mathcal{E}} \exp\left(-\frac{2}{3\,\mathcal{E}}\right); \qquad P(t) = \exp\left(-\frac{\Gamma\, t}{\hbar}\right). \tag{14}$$

However, there are corrections to the exponential decay especially at short times. We have represented in Figure 1, for three values of the electric field, the survival probabilities for short times ($t < 400$ a.u.) and the corresponding lineshapes (spectral densities). We have not represented the long-time dominant exponential decay which corresponds to times much greater ($\simeq 10^{55}$ a.u.) than 400 a.u. The choice of a unique time scale in Figure 1 ($t \leq 400$ a.u.) allows us to compare for very short times the non-expotential regimes which last 10^6, 2×10^3, 4×10^2 a.u. for the fields $\mathcal{E} = 0.005$, 0.01 and 0.02 a.u., respectively. Since we focused on the first oscillations of the survival probability we have not represented the full transitory regimes. In the three cases the survival probability oscillates. Note, that the amplitudes of these oscillations are small. The origin of these oscillations is easily found by examining the lineshapes on the right of the figure. Clearly, the resonances arising from the states $2s$ and $2p$ participate to the dynamics. It can be checked that the period of the oscillations is approximatively $T = 2\pi\,\hbar/\Delta \simeq 17$ a.u., Δ being the energy difference between the ground state $1s$ and the two lowest excited states $2s$ and $2p$.

A deeper understanding of the short-time dynamics may be found by considering the dominant terms of the Green's function

$$G(z) = \frac{f_{1s}}{z - \mathcal{E}_{1s}} + \frac{f_1}{z - \mathcal{E}_1} + \frac{f_2}{z - \mathcal{E}_2} + ... \tag{15}$$

$\mathcal{E}_{1s} = E_{1s} - \mathrm{i}\Gamma_{1s}/2$ is the complex energy of the resonance 1s and $f_{1s} \simeq 1$ is the corresponding oscillator strength. The energies $\mathcal{E}_k = E_k - \mathrm{i}\Gamma_k/2$ ($k = 1, 2$) are the energies of the resonances arising from the states $2s$ and $2p$. These

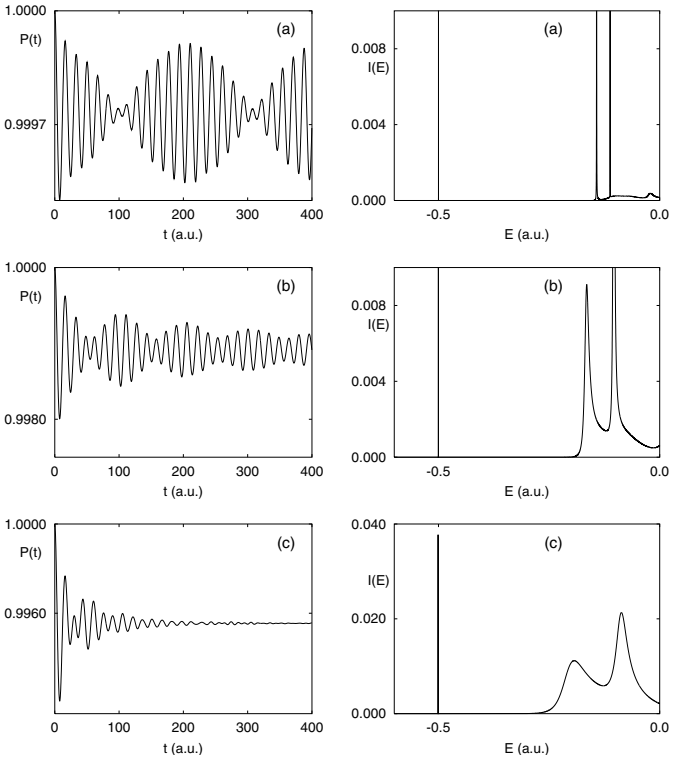

Fig. 1. *Weak coupling.* The survival probabilities $P(t)$ (2) and the lineshapes $I(E)$ (3) are represented on the left and on the right, respectively. (a) $\mathcal{E} = 0.005$, (b) $\mathcal{E} = 0.01$, (c) $\mathcal{E} = 0.02$ (atomic units).

energies are in agreement with those published in [9]. The oscillator strengths f_1 and f_2, which are responsible for the short-time dynamics, are much smaller than 1, for example, $|f_1| = 4 \times 10^{-5}$ and $|f_2| = 5 \times 10^{-5}$ in case (a). The order of magnitude of the duration of the non-expotential regime is approximatively given by the inverse of the width of the $2s$–$2p$ resonances. Since their lifetime is $\tau \simeq 10^6$ a.u. in case (a), the dynamics is reversible within the range of time [0–400 a.u.]. The survival probability displays regular quantum beats, the period of which is $2\pi\hbar/(E_2 - E_1) \simeq 200$ a.u. In cases (b) and (c), the lifetimes of the resonances are $\tau = 1000$ a.u. and 100 a.u., respectively. It results that globally the short-time dynamics displays an irreversible evolution. We will now show that the oscillations observed at low fields progressively disappear by increasing the amplitude of the electric field.

3.2 Intermediate coupling (0.02 a.u. $< \mathcal{E} <$ 0.1 a.u.)

We have plotted in Figure 2 the survival probabilities (on the left) and the lineshapes (on the right) for three values of the electric field, under, near and above the critical value $\mathcal{E} = 0.0625$ a.u., which corresponds to the disappearance of the tunneling regime. The oscillations disappear progressively when the electric field increases from $\mathcal{E} = 0.04$ a.u. in (a) to $\mathcal{E} = 0.08$ a.u. in (c). The extinction of the transitory oscillations is directly related to

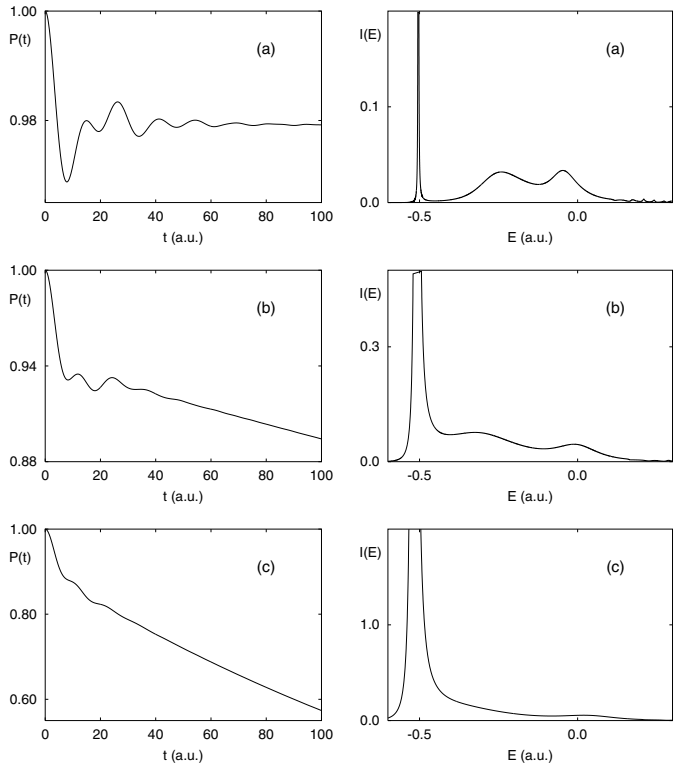

Fig. 2. *Intermediate coupling.* The survival probabilities $P(t)$ (2) and the lineshapes $I(E)$ (3) are represented on the left and on the right, respectively. (a) $\mathcal{E} = 0.04$, (b) $\mathcal{E} = 0.06$, (c) $\mathcal{E} = 0.08$ (atomic units).

the disappearance of the $2s$–$2p$ resonances as autonomous objects. The double bump still present in the lineshape (a) has disappeared in (c) which displays a broad asymmetrical profile. Note, that for $\mathcal{E} = 0.08$ a.u., case (c), the agreement between our survival probability and the full line curve in Figure 1 of [2] is perfect.

3.3 Strong coupling ($\mathcal{E} \gg 0.1$ a.u.)

For fields much higher than the critical value $\mathcal{E} = 0.0625$ a.u. the transitory regimes disappear. Broad lineshapes lead to decays which look more Gaussian than Lorentzian (Fig. 3). For these extremely high electric fields the internal Coulombic forces are of the same order of magnitude as the external field forces. The hydrogen atom is not any more a long-lived resonance but an extremely-short-lived state whose lifetime is about 1 a.u. $\simeq 10^{-17}$ s.

Figure 4 represents the survival probability (logarithmic scale) as a function of t (a) and of t^2 (b). The representations of the survival probability (a) and (b) are roughly linear, which confirms that the process is neither purely Lorentzian nor purely Gaussian. However, for times $t < 1$ a.u., the logarithm of $P(t)$ is dominated by a term proportional to t^2. In both cases the survival probabilities are depicted for two values of the rotation angle θ: 0.02 (full lines) and 0.04 (dotted lines). The curves are

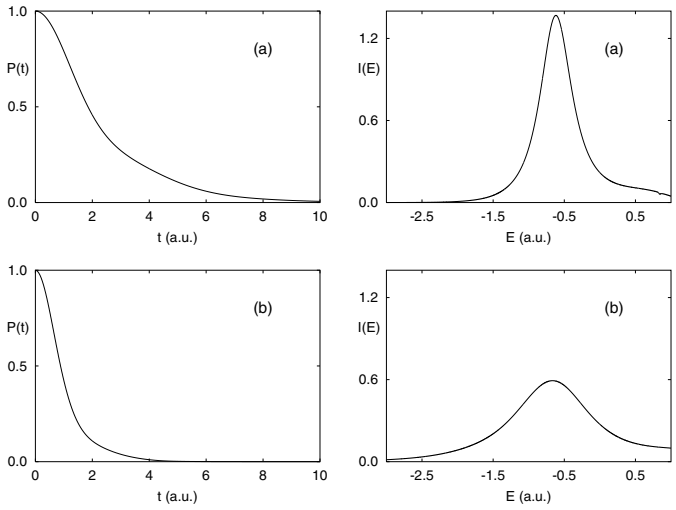

Fig. 3. *Strong coupling.* The survival probabilities $P(t)$ (2) and the lineshapes $I(E)$ (3) are represented on the left and on the right, respectively. (a) $\mathcal{E} = 0.5$, (b) $\mathcal{E} = 1.0$ (atomic units).

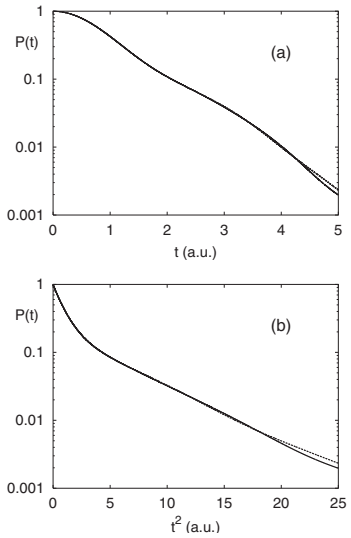

Fig. 4. *Survival probability* $\mathcal{E} = 1$. (a) Survival probability $P(t)$ (2) as a function of t. (b) Survival probability $P(t)$ (2) as a function of t^2 (atomic units). Full lines: $\theta = 0.2$; dotted lines: $\theta = 0.4$; θ is the rotation angle of the complex scaling operator S in (9).

almost identical which proves the independence of the dynamical observables on the parameters of the numerical calculation. On the other hand, the complex energies and the oscillator strengths vary with θ in a large extend. This result is not surprising: for very high field the usual concept of resonance becomes irrelevant and has to be replaced by the concept of short-lived state. Finally, we note that the mean duration of the ionization varies from 10^{55} a.u. ($\simeq 10^{48}$ s) for $\mathcal{E} = 0.005$ a.u. in Figure 1 to 1 a.u. ($\simeq 10^{-17}$ s) for $\mathcal{E} = 1$ a.u. in Figure 3, which represents a change of 55 order of magnitude for the full irreversible process!

3.4 Discussion

The results presented above display large non-expotential decays. Non-expotential decays and irreversibility have been largely investigated for many years and there is a huge literature on the subject. The theory predicting corrections to exponential decay may be found in the complement C_{III} of [11]. For very short times the probability of remaining in the initial state does not decrease linearly with t but quadratically. In addition, assuming that the range of energy of the continuum is [0–∞], the decay is less rapid than an exponential decay for very long times ($t \gg \hbar/\Gamma$, Γ being the width of the resonance) (see complement A_{III} in [11]). Various aspects of non-exponential decays can be found in [12,13]. In agreement with the theory, for very short times, the decay rate varies quadratically with t in the whole range of the electric field investigated [0.005–1 a.u.]. However, this result is not significant since, for under- the ionization barrier regime ($\mathcal{E} < 0.06$ a.u.), the dynamics for very short times is largely dominated by transitory oscillations (see Figs. 1 and 2). It is also interesting to compare our results with those found for autoionizing systems such as the He^- $1s2p^2$ ^4P or the Li^- $1s^22s2p$ $^3P^0$ shape resonances [14–16]. For a well isolated resonance ($\mathcal{E} < 0.06$ a.u. for the atom H) a transitory non-expotential decay always precedes the exponential decay. Contrary to many-electron systems, we have not observed any departure from exponential decay for very long times. This different behaviour comes from the very nature of the continuum. For the hydrogen atom, the external electric field generates a continuum of states whose energy extends from $-\infty$ to ∞ whereas for auto-ionizing states the continuum associated with the free electron starts at the energy threshold. This latter constraint on the energy is responsible for the departure from exponential decay for very long times. However, these non-expotential decays are so short that we may conclude that the hydrogen atom and many-electron systems provide similar results. In particular, the dynamical regimes for auto-ionizing states do not seem to depend significantly on the electronic correlation.

Up to now we have not discussed the choice of the ground state of the hydrogen atom as the initial state. We may ask whether it is possible to prepare a 1s state at $t = 0$ by switching on suddenly an external electric field? We have presented the solution of a well defined problem of initial condition, but is there any relationship between the mathematical formalism and the physical reality? The problem of the definition and of the calculation of the initial state has been addressed for many years especially for auto-ionizing states [17]. The initial state may be determined by variational calculations which satisfy some criterion of localization. The external electric field cannot be applied instantaneously. The experimental process is adiabatic and the atom polarizes continuously while increasing the field. Consequently, it seems more reasonable to consider as initial state the polarized state

$$|\phi\rangle = |1s\rangle - 2\mathcal{E}|p\rangle \quad \text{(a.u.)}. \tag{16}$$

$|p\rangle$ is the doorway state of angular symmetry $l = 1$ obtained by multiplying the ground state by the coordinate z of the electron [4]. Expression (16) was derived by elementary perturbation theory. We have performed some numerical studies by starting from $|\phi\rangle$ as the initial state. As expected, the pre-expotential regime, at short times, is deeply altered. Although $|\phi\rangle$ keeps a localized character, it is not, from a physical point of view, a satisfactory initial state since the electric field continuously varies with time. It results that for getting the response of the atom initially in the ground state to the electric field, one should solve the time-dependent Schrödinger equation with a time-dependent Hamiltonian. This is clearly outside the scope of this paper. In addition, it may be conjectured that the non-expotential decays will remain outside the experimental observation. Nicolaides [13] argues that "... resonance states close to threshold are good candidates for non-expotential decay...". We are far from these conditions in the ground state of the hydrogen atom.

4 Ionization from the lowest excited states

Ionization from excited states is worthwhile to study since large oscillations may appear which do not exist for the ground state. These oscillations arise from the degeneracies of the spectrum of the hydrogen atom. We have limited our study to the two lowest excited states $2s$ and $2p_z$ (hereafter denoted $2p$). The lowest linear Stark effect generates two resonances whose approximative wave functions at low field are

$$|+\rangle = \frac{1}{\sqrt{2}}(|2s\rangle + |2p\rangle), \tag{17}$$

$$|-\rangle = \frac{1}{\sqrt{2}}(|2s\rangle - |2p\rangle). \tag{18}$$

These resonances have been extensively investigated. Here we are interested in the dynamics of ionization starting from excited states which are linear combinations of $|2s\rangle$ and $|2p\rangle$. We have represented in Figures 5 and 6 the survival probabilities (on the left) and the lineshapes (on the right) proceeding from the initial states $|2s\rangle$ and $|+\rangle$ for three values of the electric field. Similar results (not discussed here) would be obtained for ionization from the initial states $|2p\rangle$ and $|-\rangle$.

As expected, for a two-level systems, the dynamics is characterized by damped oscillations (Fig. 5). The occupation numbers of the states $|2s\rangle$ and $|2p\rangle$ are represented by full and dotted lines, respectively. The damping increases from (a) to (c) with the increase of the electric field. In (a) the oscillations are reversible at the time scale of 400 a.u. whereas the decays in (b) and (c) are governed by the lifetimes $\tau_- = \hbar/\Gamma_-$ and $\tau_+ = \hbar/\Gamma_+$ of the two resonances whose complex energies $\mathcal{E}_-$ and $\mathcal{E}_+$ appear in the two dominant terms of the Green's function

$$G(z) = \langle 2s|\frac{1}{z-H}|2s\rangle = \frac{f_-}{z-\mathcal{E}_-} + \frac{f_+}{z-\mathcal{E}_+} + ... \tag{19}$$

As expected, $|f_-| \simeq |f_+| \simeq 1/2$. The widths of the resonances observed in the lineshapes are inversely proportional to the decay time. The lifetime of the metastable

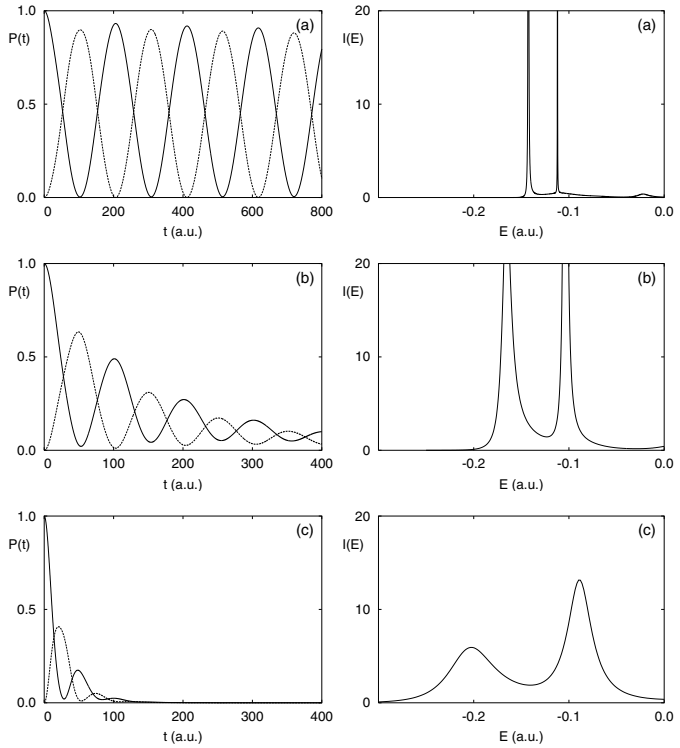

Fig. 5. *Ionization from the* $|2s\rangle$ *state.* The survival propabilities $P(t)$ (2) and the lineshape $I(E)$ (3) are represented on the left and on the right, respectively (full lines). The occupation of the state $|2p\rangle$ is represented with dotted lines. (a) $\mathcal{E} = 0.005$, (b) $\mathcal{E} = 0.01$, (c) $\mathcal{E} = 0.02$ (atomic units).

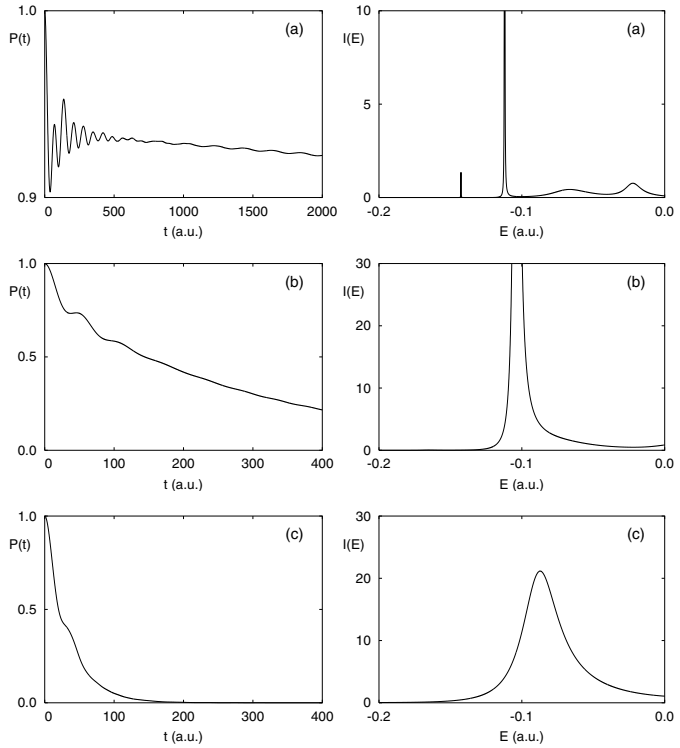

Fig. 6. *Ionization from the* $|+\rangle$ *state.* The survival propability $P(t)$ (2) and the lineshape $I(E)$ (3) are represented on the left and on the right, respectively. (a) $\mathcal{E} = 0.005$, (b) $\mathcal{E} = 0.01$, (c) $\mathcal{E} = 0.02$ (atomic units).

state $2s$ and the lifetime of the state $2p$ corresponding to spontaneous emission were not considered here since they are much greater than the lifetimes of the resonances within the range of the electric field investigated. In Figure 6 ionization starts from the initial state $|+\rangle$ which is a resonance. Consequently, the large oscillations observed in Figure 5 have disappeared and the resonance decays almost exponentially. In case (a) the transitory oscillation of small amplitude are quite similar to those observed for the ground state (see Fig. 1c).

In contrast with small amplitude oscillations arising from the ground state (Fig. 1), large amplitude oscillations are found in Figure 5. Does it mean that these oscillations could be observed? Their lifetimes 400 a.u $\simeq$ 10 fs is sufficient for an experimental detection but how to prepare these resonances in a very high static electric field? Switching on a static electric field requires typically 1 ns which is much larger than the resonance lifetimes ($\simeq$ 10 fs). This means that these time-dependent phenomena probably do exist in highly ionized media but may not be observable in the laboratory.

5 Conclusion

We have presented an overall treatment of the problem of the decay of the ground state of an hydrogen atom in an external static electric field for weak (under the barrier) and strong (above the barrier) electric fields. Our results complete those previously found by Scrinzi and Geltman. We have systematically investigated the departures from exponential decay within an extended range of electric fields. At low field the oscillating transitory regimes were interpreted in term of excitation of the lowest resonances above the ground state. At higher field, the transitory regimes disappear and the decays look more Gaussian than Lorentzian. In a complementary study we have also investigated various dynamical regimes arising from the lowest excited states. It is noteworthy that the hydrogen atom, as soon as it is put into a static electric field, may provide such an extended set of reversible and irreversible time-dependent phenomena. This means that irreversibility is already present within the dynamics of the simplest atom. The various decay regimes discussed in this paper surely exist although they might not be directly observable. At all the steps of our study we have kept an equal balance between the variables energy and time, as suggested by the dual role played by the Hamiltonian in quantum mechanics [18]. This point of view might be fruitful for computing and understanding the physics of many-electron systems.

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