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Relativistic effects in the time evolution of an one-dimensional model atom in a laser pulse

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Abstract. We define 1D Volkov states as solutions of the one-dimensional Dirac equation in a time dependent electric field, similar to the Volkov solutions in the three dimensional case. They are eigenspinors of the momentum operator and reduce in the absence of the field to free solutions of positive or negative energy. Then we add a time independent attractive Gausssian potential and, by integrating the Dirac equation for a laser pulse of Gaussian shape, we determine the state which coincides initially with the ground state of the system in the absence of the electric field. Our main objective is the study of the population dynamics on the Volkov states during the pulse action. For different values of the laser pulse intensity and two values of the potential depth, we find that the Volkov states which evolve from free solutions of negative energy are practically not populated, in contrast to the population on free negative energy states.

PACS. 03.65.Pm Relativistic wave equations – 32.90.+a Other topics in atomic properties and interactions of atoms with photons

1 Introduction

The impressive advances in laser technology have given access to intensities at which the ponderomotive energy of the electron becomes of the same order of magnitude with its rest energy, making imperious the need for a relativistic description of atom-laser interaction. The search for different approaches and methods of calculations is reflected in many publications and in the recent ample review paper by Salamin et al. [1]. As emphasised by Maquet and Grobe [2], the relativisitic quantum mechanics of atoms in super-intense laser field faces many challenges. Recent calculations [3] have shed light on the correct way of interpreting concrete results using quantum electrodynamics.

In a calculation based on Dirac equation, both retardation and relativistic effects are automatically taken into account. There is a regime of field intensities and electron energies in which the retardation effects only matter. A calculation beyond the nonrelativistic dipole approximation takes into account the magnetic field influence on the electron behaviour. It was suggested in the first calculations [4,5], and confirmed afterwards [6–9], that the main effect of the magnetic field, taken into account through the inclusion of the non-dipole terms, is to push the electron along the field propagation direction such that at the end of the laser pulse it is left very far from the nucleus, the consequence being the atomic destabilization.

To our knowledge, the 3D Dirac equation for an atom in a laser field was in fact not integrated numerically up to now. Only a few 1D (Protopapas et al. [10], Kylstra et al. [11], Lenz et al. [12]) and 2D simulations [13–15] have been published. For the realistic three dimensional case, although several algorithms were proposed [16–18], only results for the free electron in a plane wave laser field exist [19]. A promising approximation scheme was proposed by Krstic and Mittelman [20], in order to transform the solving of the Dirac equation in a simpler numerical problem.

One-dimensional time-dependent Schrödinger equation was a useful tool for the description of atom-laser interaction leading to a qualitative description of phenomena as above-threshold ionization [21] and to exploratory studies of dynamic stabilization [22]. For a relativistic description of atom-laser interaction the use of one-dimensional Dirac equation is plagued by the fact that one can not take into account the position dependence of the external field, so automatically retardation effects are ignored. It has the particularity of revealing only relativistic effects.

Well aware of the limitations introduced by a study based on 1D Dirac equation, we present here results of several calculations based on it, with the hope that some of the features of the time evolution of the system could be qualitatively extended to the 3D case. One of the problems, that was addressed in the 1D case by Kylstra et al. [11], was the coupling between positive and negative energy states induced by the external field. The conclusion was that at relativistic intensities the negative energy states gets significantly populated during the action of an

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intense laser pulse, so, in order to obtain an accurate description of the time evolution of a spinor wavepacket, the contribution of free negative energy solutions can not be neglected.

In the present paper we analyze the evolution of the electron in a different way than was done in the past. For the electron in the presence of an electric field, we define particular solutions (named Volkov solutions) of 1D Dirac equation which evolve from solutions of the free Dirac equation of given momentum. Although, in contrast with the 3D case, an analytical expression of these solutions can not be found, some general properties, as the completeness and orthogonality remain true. We study the transfer of population between such states, determined numerically, for particular initial state and show that, unlike for the case of free solutions, the coupling between Volkov solutions is much reduced. This shows that these states form a better suited basis to study the time evolution of the state spinor. Our main conclusion is that if at the initial moment negative energy states are practically not present in the wavespinor, and if the atomic potential is not too deep, then the Volkov states originating from negative energy free solutions can be safely neglected.

The one-dimensional Volkov solutions are defined in Section 2. Numerical results are presented in Section 3, based on the integration of the 1D Dirac equation for a model atom with potential energy given in equation (9) interacting with an external electric pulse described by equation (10). For a selected solution of the 1D Dirac equation, we calculate the total probabilities to find the electron in positive and negative energy free states and the populations in each of the two types of Volkov states. The results presented in Figures 2 and 3 illustrate the influence of the laser intensity and of the potential strength on the population transfers. Our conclusions are resumed in Section 4. Details on the numerical method used for the calculation of Volkov solutions and for the integration of the Dirac equation in the presence of a potential are given in the Appendix.

2 The one-dimensional Dirac equation in an external electric field

The one-dimensional Dirac equation for an electron interacting with a potential $V(x)$ and an external time-dependent electric field $\mathcal{E}(t)$ described by

$$A(t) = -\int^{t} \mathcal{E}(t')dt'$$

reduces to two uncoupled two components equations of the form [11]

$$i\frac{\partial \Phi}{\partial t} = \left\{c\sigma_x[P_x + A(t)] + V(x) + c^2\sigma_z\right\}\Phi, \qquad (1)$$

such that it is relevant to study only one of them. In the above equation σ_x and σ_z are the Pauli matrices, and Φ is a two component spinor and atomic units are used.

In the particular case of the free electron ($V(x) = 0$, $\mathcal{E}(t) = 0$) equation (1) has the well-known particular solutions

$$\chi_{\pm}(p;x,t) = \frac{1}{\sqrt{2\pi}}\exp[i(px \mp Et)]v_{\pm}(p), \;\; p \in (-\infty,\infty), \qquad (2)$$

with

$$v_{+}(p) = \frac{1}{\sqrt{2E(E+c^2)}}\begin{pmatrix} E+c^2 \\ cp \end{pmatrix}$$
$$v_{-}(p) = \frac{1}{\sqrt{2E(E+c^2)}}\begin{pmatrix} -cp \\ E+c^2 \end{pmatrix} \qquad (3)$$

and $E = c\sqrt{p^2+c^2}$. The spinors $\chi_{+}(p;x,t)$ and $\chi_{-}(p;x,t)$ are positive and, respectively, negative frequency solutions. They are also eigenvectors of the operator P_x, corresponding to the eigenvalue p. The ensemble of solutions $\chi_{\pm}(p;x,t)$ form a complete and orthonormalized set.

In the state described by a spinor $\Psi(x,t)$, the total probability to find the electron in a positive/negative energy free state is given by

$$P_{\pm}(t) = \int_{-\infty}^{\infty} dp|v_{\pm}^{\dagger}(p)\tilde{\Psi}(p,t)|^2, \qquad (4)$$

where $\tilde{\Psi}(p,t)$ is the Fourier transform of the spinor $\Psi(x,t)$ and $v_{\pm}^{\dagger}(p)$ are the transpose conjugate of $v_{\pm}(p)$.

We *define* the one-dimensional Volkov functions as the particular solutions of the Dirac equation (1) in the absence of the atomic potential that at the initial moment t_0, when the external field is supposed to be zero, reduce to the free solutions (2). We call these solutions one-dimensional Volkov solutions because a correspondence exists with the true Volkov functions [23], which are exact solutions of the 3D Dirac equation for a charged particle interacting with an arbitrary electromagnetic pulse with a fixed direction of propagation. In the absence of the electromagnetic field the three-dimensional Volkov solutions [23], reduce to free solutions. The properties of the 1D Volkov solutions are briefly presented here; some of them are similar to those of the usual three dimensional Volkov solutions.

From the definition, it follows that in the one-dimensional Dirac equation case, there is a one-to-one correspondence between Volkov and free solutions, expressed by

$$\psi_{\pm}(p;x,t) = U(t,t_0)\chi_{\pm}(p;x,t_0), \qquad (5)$$

where $U(t,t_0)$ is the evolution operator associated to the Dirac equation (1) for $V = 0$. As the momentum operator P_x commutes with the Dirac Hamiltonian in equation (1), the Volkov solutions are at any moment t eigenspinors of this operator,

$$\psi_{\pm}(p;x,t) = \frac{1}{\sqrt{2\pi}}\nu_{\pm}(p,t)\exp(ipx), \;\; p \in (-\infty,\infty) \qquad (6)$$

where the spinor $\nu(p,t)$, unlike in the three dimensional case, is independent on the position. Although its evolution equation,

$$i\frac{d\nu_{\pm}}{dt} = \left\{c\sigma_x[p + A(t)] + c^2\sigma_z\right\}\nu_{\pm}(p,t), \qquad (7)$$

is much simpler than the corresponding three-dimensional one, it has no analytical solution. It is also useful to notice that the spinors $\nu_{\pm}(p,t)$ are the Fourier transforms of the Volkov spinors $\psi_{\pm}(p;x,t)$.

Volkov solutions are classified in two categories, according to their origin from positive or negative free states. Even if we can not find the explicit expressions for the one-dimensional Volkov solutions, one can assert that they form an orthonormal and complete set, due to the unitarity of the evolution operator. As a consequence, the Volkov solutions form a basis set, and any spinor $\Psi(x,t)$ can be written as a continuous linear superposition of them. As in the case of the free solutions (4), we can define the total probability to find the particle in Volkov states originating from positive or negative energy free solutions

$$\Pi_{\pm}(t) = \int_{-\infty}^{\infty} dp|\nu_{\pm}^{+}(p)\tilde{\Psi}(p,t)|^2. \qquad (8)$$

The physical meaning of $\Pi_{-}(t)$ was analyzed in the paper of Krekora et al. [3].

3 Numerical results

We consider an one-dimensional model atom described by the potential energy

$$V(x) = -V_0 \exp\left(-\frac{x^2}{a^2}\right), \qquad V_0 > 0, \qquad (9)$$

interacting with the laser pulse of Gaussian shape described by the potential $A(t)$,

$$A(t) = A_0 \exp\left[-\left(\frac{1.1774t}{\tau_p}\right)^2\right]\sin(\omega t), \qquad T = \frac{2\pi}{\omega}; \qquad (10)$$

with frequency $\omega = 1$ au and full width at half maximum $\tau_p = 1$ cycle.

In the numerical calculation we take the parameter describing the width of the atomic potential $a = 2$ au, and, in order to study the effect of the potential depth on the time evolution of the system, two values of the potential depth: $V_0 = 1$ au, for which the ground state energy is $E_g = -0.7$ au and, respectively, $V_0 = 5$ au, for which $E_g = -4.2$ au. The initial state of the system, at a moment before the beginning of the pulse, is chosen as the ground state of the isolated atom. We present numerical results for the peak value of the potential $A_0 = 25$ au, for which the relativistic effects are small, and $A_0 = 50$ and 100 au, values located outside the validity range of the non-relativistic approximation.

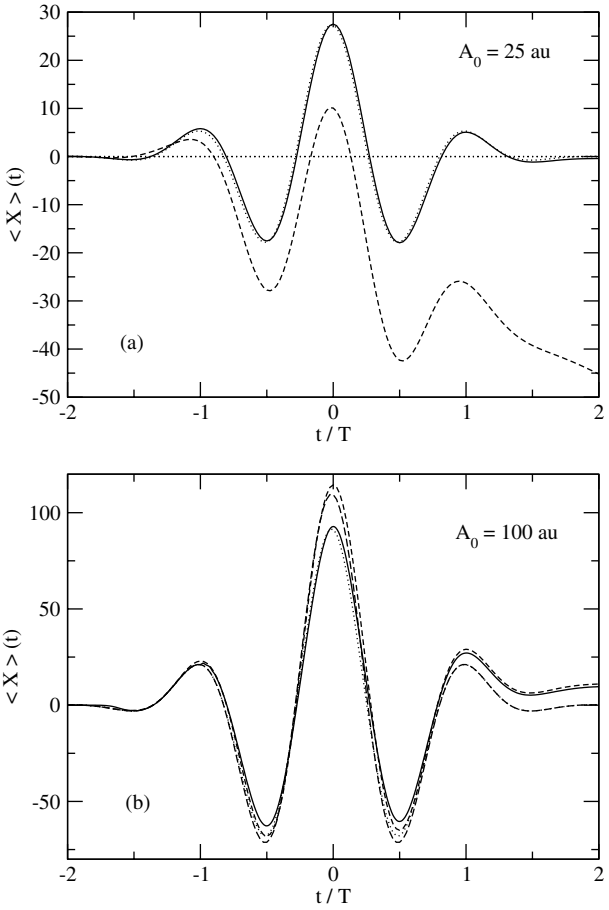

Fig. 1. (a) Expectation values of position calculated from the Dirac equation for $V_0 = 1$ au (full line) and $V_0 = 5$ au (dashed line) and classical trajectory of the free electron in the laser pulse (dotted line). (b) Expectation values of position for $V_0 = 1$ au, calculated from the Dirac equation (full line) and Schrödinger equation (dashed line) and classical relativistic (dotted line) and non-relativistic (long-dashed line) trajectory.

In order to compare the relativistic and non-relativistic results, we have also integrated the Schrödinger equation for the same system parameters, and we have compared the expectation value of the position operator X calculated within relativistic ($\langle X\rangle_D(t)$) and non-relativistic ($\langle X\rangle_S(t)$) approach. For $A_0 = 25$ au the relativistic and non-relativistic results are identical. In Figure 1a the expectation values are presented as functions of time, for $V_0 = 1$ au (full line) and $V_0 = 5$ au (dashed line). With dotted line is represented the classical trajectory of the free electron in the laser pulse,

$$\alpha(t) = \int^{t} d\tau A(\tau). \qquad (11)$$

One can see that, for $V_0 = 1$ au, the electron moves along the classical trajectory, which is a consequence of the fact that the atomic potential is negligible with respect to the external field. By contrast, in the case $V_0 = 5$ au, the effect of the atomic potential is important, and $\langle X\rangle(t)$ and $\alpha(t)$

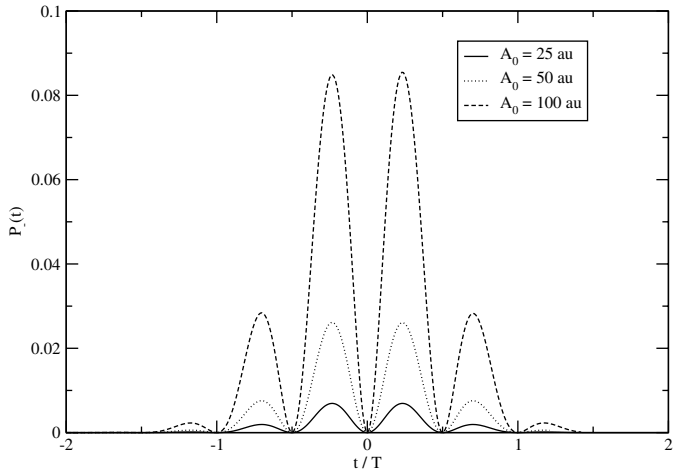

Fig. 2. The function $P_{-}(t)$ in equation (4) for $V_0 = 1$ au and three values of A_0, as indicated in the legend.

are very different. In order to understand this result we start from the Ehrenfest theorem

$$\langle X\rangle(t) = \alpha(t) - \int^{t} dt' \int^{t'} dt'' \left\langle \frac{dV}{dx} \right\rangle (t''). \qquad (12)$$

In the case $V_0 = 1$ au, the second term in the previous equation can be neglected, and one obtains $\langle X\rangle(t) \approx \alpha(t)$, while for $V_0 = 5$ au this term is responsible for the differences observed in Figure 1a. In Figure 1b we have represented for $A_0 = 100$ au and $V_0 = 1$ au: $\langle X\rangle_D(t)$ (full line), $\langle X\rangle_S(t)$ (dashed line), $\alpha(t)$ (dotted line) and the classical relativistic trajectory [11] (long dashed line),

$$\alpha_r(t) = \int^{t} d\tau \frac{A(\tau)}{\sqrt{1 + A^2(\tau)/c^2}}. \qquad (13)$$

In this case, the effect of the atomic potential is again negligible with respect to the laser field, and $\langle X\rangle_D(t)$ is similar to $\alpha_r(t)$, while $\langle X\rangle_S(t)$ is similar to $\alpha(t)$. However, we must note that the difference between them is very small.

Next, we have calculated $P_{\pm}$ and $\Pi_{\pm}$, defined in equations (4) and (8), respectively, for the two values of the potential $V_0 = 1, 5$ au and for three values of the external field $A_0 = 25, 50, 100$ au. Our results show that $P_{\pm}$ are practically identical at different V_0 and fixed A_0, but have a strong dependence on the field intensity. In Figure 2 the function $P_{-}(t)$ is presented for $A_0 = 25, 50, 100$ au. One can see that $P_{-}(t)$ increases strongly with A_0, reaching a maximum value of about 0.09 for $A_0 = 100$ au. $P_{+}(t)$ can be calculated from the relation $P_{+}(t) = 1 - P_{-}(t)$.

In Figure 3 the function $\Pi_{-}(t)$ is presented for the same values of the external field intensity as before and of the potential depth ((a): $V_0 = 1$ and (b): $V_0 = 5$ au). Unlike in the previous case, the projection of the wavespinor on the Volkov solutions originating from negative energy solutions is extremely small even at the largest value of the field intensity. In spite of this, we are able to understand the structure of Π_{-} as function of time, based on

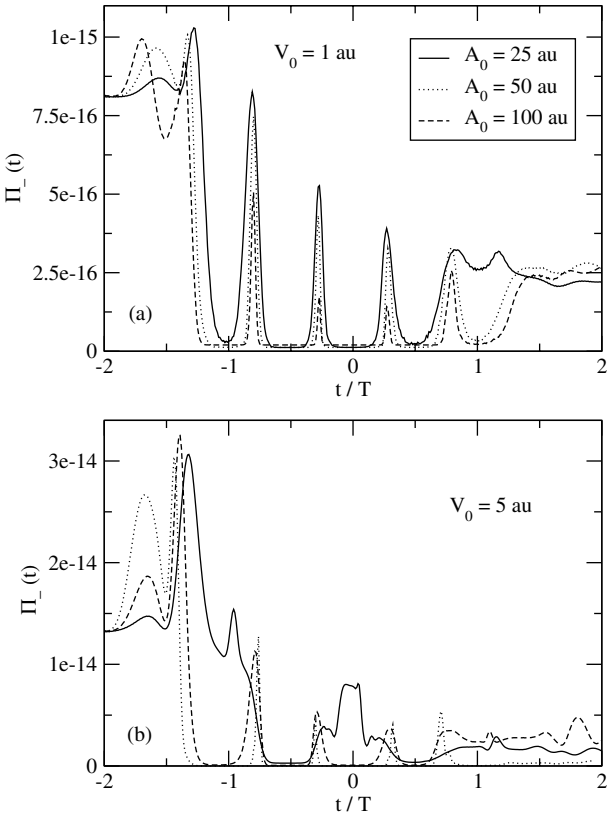

Fig. 3. The function $\Pi_{-}(t)$ in equation (8) for three values of A_0, and two values of the potential depth V_0.

the information on the electron trajectories described before. An important difference between P_{-} and Π_{-} is that the time-dependence of $\Pi_{-}(t)$ is influenced also by the atomic potential depth. For $V_0 = 1$ au $\Pi_{-}(t)$ has maxima of the same order of magnitude as the initial value $\Pi_{-}(-\infty)$, at moments near $t = (1/4 + n/2)T$ with n integer, which are the moments when the electron is located near the nucleus (see Fig. 1). This can be easily understood since the transfer of population between Volkov solutions takes place only due to the interaction with the atomic potential. Between these sharp maxima the value of $\Pi_{-}(t)$ is almost constant, and much reduced. We also notice that higher the field intensity, sharper the maxima are; the explanation is that for higher field intensity the electron crosses the region around nucleus with large speed, so the time spent near the origin is smaller. The situation is similar for the case $V_0 = 5$ au; however, some differences exist. First, we notice that the initial value of Π_{-} is larger than in the previous case, which is due to the fact that the binding energy of the ground state is larger. The general features for $A_0 = 50$ and 100 au are the same as in the previous case: they have peaks localized around the same positions as for $V_0 = 1$ au, and their width and height have the same behaviour with A_0. For $A_0 = 25$ au, the behaviour of $\Pi_{-}(t)$ is very different, however: it has a peak around $t = -T$, and a wide maxima near the $t = 0$. This situation appears because the trajectory followed by the electron is different in this case. From Figure 1 one

can see that, unlike in the previous situations, the trajectory crosses the origin near those two moments, and, as a consequence a transfer of population takes place. However, we must keep in mind that during the interaction with the pulse the wavepacket spreads too, and at $A_0 = 25$ au the amplitude of oscillation is relatively small, such that during the second part of the pulse the wavespinor is always overlapping with the nucleus.

Our results show that, unlike the negative energy free states, the Volkov states originating from them are practically not populated during the interaction with the external field, even at relatively high external field intensity. The transfer of population between them takes place only at the moments when the wavepacket overlaps with the nucleus, and, at fixed laser intensity, is more important for deeper atomic potentials. From this we can infer that at least for not too deep potentials and if the initial state is a low energy one, it should be possible to numerically solve the Dirac equation in a basis set consisting only in Volkov states originating from positive energy solutions. The same conclusion should apply also for the three dimensional case; in fact, this case should be even more convenient from this point of view, as the electron is pushed away from the nucleus due to the retardation effects, so the interaction with the nucleus is even less important. We mention also that in the 3D case the solving of the Dirac equation in a Volkov state basis is favored by the fact that the Volkov solutions have known analytical expression.

4 Conclusions

In conclusion, we have numerically integrated the one-dimensional Dirac equation for an atom interacting with a laser pulse. We have calculated the expectation value of the position operator X as a function of time, and we have compared the results with the corresponding non-relativistic ones. The comparison shows that even at the highest intensity studied the relativistic effects on $\langle X \rangle$ are extremely small.

We have also studied the population on negative energy free states and we have seen that it practically does not depend on the atomic potential depth, but increases fast with the increasing of the laser intensity. By contrast, the population on Volkov states originating from negative energy free states is extremely small, and do not exceed the value at the initial moment. The transfer of population takes place only as a consequence of the interaction of the wavepacket with the atomic potential, at the moments when the two overlap.

We have suggested the possibility to analyze in a similar way a solution of 3D Dirac equation.

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Appendix A: Details on the numerical calculation

The numerical integration of the one-dimensional Dirac equation in the presence of the atomic potential was performed using the split-operator method. The most important complication arising in this case is related to the fact that due to the presence of the term c^2 in the Hamiltonian the time step δt must be chosen such that $c^2 \delta t \ll 1$ [11], which gives a very small value for δt of the order 10^{-8} au, and, as a consequence, the numerical code will be extremely slow. In order to save some running time we made use of the fact that the Hamiltonian depends on time only due to the field $A(t)$ which changes in time with the frequency ω of the order of unity. So the same value of A can be used for several consecutive time-steps, and the propagator could be recalculated only once for several consecutive time-steps.

In the numerical examples presented in Section 3 the initial state is chosen the ground state of the unperturbed atom, whose knowledge is required with a very good accuracy. The calculation was performed using a method proposed by Muller [24]: using as initial condition an approximation of the ground state, one integrates the Dirac equation for the electron in the atomic potential, and the eigenstate we are looking for is identified with the time average

$$\langle \Psi(x,t) \exp(iE_0 t) \rangle_\tau, \tag{A.1}$$

where E_0 is an approximation of the ground state energy and the time average must be taken along a sufficiently long time-interval τ such that the convergence is reached.

In order to numerically calculate the Volkov solutions $\psi_\pm(p;x,t)$ we must in fact solve equation (7), with the initial conditions

$$\nu_\pm(p,t_0) = v_\pm(p), \tag{A.2}$$

with $v_\pm(p)$ defined in (3). Formally, the equation can be written as

$$\nu_\pm(p,t) = U_v(t,t_0;p) v_\pm(p), \tag{A.3}$$

where $U_v(t,t_0;p)$ is the time-evolution operator associated to equation (7), and it can be easily numerically solved since the "Hamiltonian" in equation (7) is a multiplicative operator.

The accuracy of our code was checked by performing convergence tests with respect to all relevant parameters. Our conclusion is that the numerical results presented here are affected by an error of at most 1%.

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