Nuclear Instruments and Methods in Physics Research B 267 (2009) 382–385

Contents lists available at ScienceDirect

Nuclear Instruments and Methods in Physics Research B

journal homepage: www.elsevier.com/locate/nimb

Atomic ionization by a sudden momentum transfer

D.G. Arbó [a,*], K. Tőkési [b], J.E. Miraglia [c]

[a] Institute for Astronomy and Space Physics, IAFE, CC 67, Suc. 28, (1428) Buenos Aires, Argentina
[b] Institute of Nuclear Research of the Hungarian Academy of Sciences (ATOMKI), Debrecen, Hungary
[c] Department of Physics, FCEN, University of Buenos Aires, Argentina

ARTICLE INFO

Available online 13 November 2008

PACS:
32.80.Rm
32.80.Fb

Keywords:
Over-the-barrier ionization
Coulomb–Volkov
Sudden momentum transfer

ABSTRACT

We present a theoretical study of the distributions of ejected electrons as a result of the ionization of a hydrogen atom by a sudden momentum transfer. We show that the Coulomb–Volkov distorted wave theory in the impulsive limit reproduces the exact solution of the time dependent Schrödinger equation. The validity of the strong field approximation is also probed. We show that whereas classical and quantum momentum distributions right after a kick are identical, pronounced differences arise during the subsequent electron-nucleus interaction for weak momentum transfers.

1. Introduction

The Coulomb–Volkov approximation (CVA) has been widely used to describe the ionization of atoms by short laser pulses in the last decade [1–3]. The CVA is a time dependent distorted wave theory [4–6] that allows us to include the effect of the remaining core into the final state at the same approximation level as the external field. In this way, the collision dynamics due to the effects of the core potential on the detached electron can be directly probed. Several studies have been performed so far to determine the accuracy of the CVA [7,8].

On the other hand, in the last two decades there was a great revival of the classical trajectory Monte Carlo (CTMC) calculations applied to atomic collisions involving three or more particles [9,10]. These approximations gain importance in those cases when higher order perturbations should be applied or many particles take part in the processes [11,12]. The CTMC method has been quite successful also in dealing with the ionization process in laser-atom collisions, when, instead of the charged particles, electromagnetic fields are used for excitation of the target.

In the present work we study the efficiency of the strong field approximation (SFA) [13], which is a variant of the CVA [14]. The electron emission spectra of a hydrogen atom excited by ultrashort pulses are calculated within the framework of CVA and a classical trajectory Monte Carlo (CTMC) method. We analytically prove that in the limit of zero pulse duration and finite momentum transfer, CVA reproduces the exact quantum mechanical electron yields [15]. Atomic units are used throughout the paper.

2. Theory

2.1. Quantum mechanical approach

We consider an atom interacting with an ultra-short pulse described through a time dependent electric field along the $\hat{\mathbf{z}}$ direction. The total Hamiltonian of the system can be written as: $H(t) = H_0 + V(t)$, where $H_0 = \mathbf{p}^2/2 - Z/r$ is the atomic Hamiltonian, Z is the atomic charge, $\mathbf{p}$ and $\mathbf{r}$ are the momentum and position of the electron, respectively, and $V(t) = \mathbf{r}\cdot\mathbf{F}(t)$ is the interaction term with the external field, $\mathbf{F}(t)$, in the gauge length. When the interaction time is short compared to the orbital time of an electron in the ground state, the field $\mathbf{F}(t)$ can be approximated as

$$\mathbf{F}(t) = -\Delta p\,\delta(t)\hat{\mathbf{z}}, \tag{1}$$

where Δp is the momentum transferred by the field. We confine our study to a hydrogen atom ($Z = 1$) initially in its ground state.

As a consequence of the interaction with the laser pulse, one electron, initially bound to the target nucleus in the state $|\phi_i\rangle$, is emitted with momentum $\mathbf{k}$ and energy $\varepsilon_f = k^2/2 (k = |\mathbf{k}|)$. Thus, the process possesses cylindrical symmetry around the polarization axis and thereby the azimuthal angle is cyclic. Electron momentum distributions can be calculated from the transition matrix as

* Corresponding author.
E-mail address: diego@iafe.uba.ar (D.G. Arbó).

0168-583X/$ - see front matter © 2008 Elsevier B.V. All rights reserved.
doi:10.1016/j.nimb.2008.10.086

$$\frac{dP}{d\mathbf{k}} = |T_{if}|^2, \tag{2}$$

where T_{if} is the T-matrix element corresponding to the transition $\phi_i \to \phi_f$, where $|\phi_f\rangle$ is the final unperturbed state. Within the CVA, T_{if} can be computed within the framework of the sudden Coulomb–Volkov (SCV) and the strong field approximation (SFA) [14].

The transition amplitude in the *prior* form within the SCV approximation is given by [7,5]

$$T_{if}^{SCV} = \lim_{t\to-\infty} \langle \chi_f^{CV-}(t)|\phi_i(t)\rangle, \tag{3}$$

where the final Coulomb–Volkov distorted wave function $\chi_f^{CV-}(t)$ can be written as [7]

$$\chi_f^{CV-}(\mathbf{r},t) = \phi_{\mathbf{k}}^-(\mathbf{r},t)\exp(iD^-(\mathbf{k},\mathbf{r},t)). \tag{4}$$

In Eq. (4), $\phi_{\mathbf{k}}^-$ is the unperturbed final state given by

$$\phi_{\mathbf{k}}^-(\mathbf{r},t) = e^{-i\frac{k^2}{2}t}\frac{\exp(i\mathbf{k}\cdot\mathbf{r})}{(2\pi)^{3/2}}\mathscr{D}_C(Z_T,\mathbf{k},t), \tag{5}$$

where $\mathscr{D}_C(Z_T,\mathbf{k},t) = N_T^-(k)\,{}_1F_1(-iZ_T/k,1,-ikr-i\mathbf{k}\cdot\mathbf{r})$. The Coulomb normalization factor $N_T^-(k) = \exp(\pi Z_T/2k)\Gamma(1+iZ_T/k)$ coincides with the value of the Coulomb wave function at the origin, ${}_1F_1$ denotes the confluent hypergeometric function, and Z_T is the electric charge of the parent ion. The Volkov phase D^- in Eq. (4) is given by [16]

$$D^{\pm}(\mathbf{k},\mathbf{r},t) = \mathbf{A}^{\pm}(t)\cdot\mathbf{r} - \mathbf{k}\cdot\int_{\mp\infty}^{t} dt'\mathbf{A}^{\pm}(t') - \frac{1}{2}\int_{\mp\infty}^{t} dt'(\mathbf{A}^{\pm}(t'))^2, \tag{6}$$

where $\mathbf{A}^{\pm}(t) = -\int_{\mp\infty}^{t} dt'\mathbf{F}(t')$ is the vector potential. In the present case $\phi_i(t)$ and $\phi_{\mathbf{k}}^-(t)$ are the solutions of the time dependent Schrödinger equation with the non-perturbed atomic Hamiltonian H_0. When we consider a sudden momentum transfer (kick) in Eq. (1) the vector potential reduces to $\mathbf{A}^{\pm}(t) = \pm\Delta\mathbf{p}\theta(\pm t)$, where θ denotes the Heaviside step function. Therefore, the Volkov phase of Eq. (6) reads

$$D^{\pm}(\mathbf{k},\mathbf{r},t) = \pm\Delta\mathbf{p}\cdot\mathbf{r}\theta(\pm t) \mp \mathbf{k}\cdot\Delta\mathbf{p}t\theta(\pm t) - \frac{1}{2}|\Delta\mathbf{p}|^2 t\theta(\pm t). \tag{7}$$

Now, when we include the Volkov phase for a sudden momentum transfer of Eq. (7) into the final distorted wave function of Eq. (4) and this latter into the SCV transition matrix [Eq. (3)], the transition probability [Eq. (2)] becomes

$$\left(\frac{dP}{d\mathbf{k}}\right)^{SCV} = |T_{if}^{SCV}|^2 = \left|\langle\phi_{\mathbf{k}}^-(\mathbf{r})|e^{i\Delta\mathbf{p}\cdot\mathbf{r}}|\phi_i(t)\rangle\right|^2, \tag{8}$$

which turns out to be equal to the exact solution of the time dependent Schrödinger equation [15]. Hence, the SCV describes the exact quantum transition probabilities when the external field is so short that can be considered as a sudden momentum transfer. This result is not valid for pulses of finite (not ultra-short) duration as it was shown in [5].

The solutions of the Hamiltonian of a free electron in the time dependent electric field, $i\frac{\partial}{\partial t}|\chi_f^-(t)\rangle = \left(\frac{p^2}{2}+V(t)\right)|\chi_f^-(t)\rangle$ are the Volkov states [16]

$$\chi_{\mathbf{k}}^{(V)-}(\mathbf{r},t) = \frac{\exp(i\mathbf{k}\cdot\mathbf{r})}{(2\pi)^{3/2}}\exp[iD^-(\mathbf{k},\mathbf{r},t) - i\varepsilon t] \tag{9}$$

which can be obtained from Eqs. (4) and (5) replacing $\mathscr{D}_C(Z_T,\mathbf{k},t)$ by 1. Inserting Eqs. (9) into (3) leads to the strong field approximation (SFA). Hence, the total transition probability within the SFA is the simple Fourier transform of the initial wave function but shifted by the magnitude $\Delta\mathbf{p}$ in the momentum space

$$\frac{dP^{SFA}}{d\mathbf{k}} = \left|\tilde{\phi}_i(\mathbf{k}-\Delta\mathbf{p})\right|^2, \tag{10}$$

where $\tilde{\phi}_i$ denotes the Fourier transform of the initial state ϕ_i. Applying the Parseval–Plancherel theorem stating that a function and its Fourier transform have the same norm, the total ionization probability within the SFA is equal to one. This result does not depend on the value of $\Delta\mathbf{p}$ showing the accuracy of the SFA for strong kicks ($\Delta\mathbf{p} \gg 1$) but also the absurd result of the SFA for the total ionization probability when $\Delta\mathbf{p}$ is small (or even zero!). Nevertheless, the SFA does predict a real physical magnitude. As the SFA neglects the effect of the Coulomb potential on the electron after the kick, it predicts the exact velocity distribution of the electron yield right after the kick (at $t = 0^+$, when no further Coulomb attraction is possible yet). This result lets us study the effect of the Coulomb potential on the electronic cloud since it is exactly calculated in the full CVA but completely neglected by the SFA.

2.2. Classical simulation

CTMC is a nonperturbative method, where classical equations of motion are solved numerically. The initial electronic state of the target atom is obtained from the microcanonical distribution. In the SFA the classical momentum distribution is shifted in Δp along the $\hat{z}$ direction and the distribution is not affected by the Coulomb potential. This is a good approximation for the case of $\Delta p \gg 1$. Within the SFA, the time evolution of a classical and quantum sudden momentum transfer is exactly the same, i.e. classical dynamics has exactly the same ionization yield as quantum mechanics. Therefore, due to the fact that the quantum and classical (in the microcanonical ensemble) initial momentum distributions are the same, the distributions also must be the same after the kick. Although the dynamics of a sudden momentum transfer is described equally by the time dependent Schrödinger equation and the Hamilton's equations, the time evolution of the motion of the kicked electron under the effect of the atomic Coulombic electric field can show significant differences.

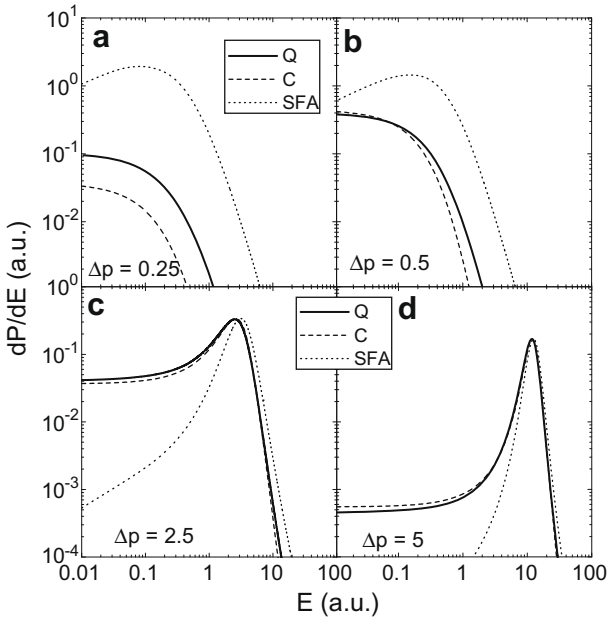

Fig. 1. Energy spectrum of H ionized by a sudden momentum transfer of kick strength (a) $\Delta p = 0.25$, (b) $\Delta p = 0.5$, (c) $\Delta p = 2.5$, and (d) $\Delta p = 0.5$. Quantum: solid line; classical: dashed line; and SFA: dotted line.

3. Results and discussion

It is known that in the case of low kick strengths (dipole or perturbative regime), quantum and classical dynamics for the atomic ionization yield predict very different outcomes. For example, for ionization of a hydrogen atom due to a sudden momentum transfer $\Delta p = 0.25$, CTMC predicts only 0.4%, whereas quantum mechanics 2%, five times higher. This behavior is known in the literature as classical suppression [15]. This effect can be observed in the energy spectrum of Fig. 1(a). When we double the kick strength ($\Delta p = 0.5$), the total classical ionization probability is 7.7%, while the quantum one is 9.6%, i.e. a factor 1.25 of difference. Although the energy spectrum is satisfactorily reproduced by classical mechanics, this is not the case for the momentum distribution. In Fig. 2 the quantal (a) and classical (b) doubly-differential momentum distribution $d^2P/dk_\rho dk_z$ of the electron yield after the same sudden momentum transfer ($\Delta p = 0.5$) are displayed. We note, that the statistical errors for the classical distribution (below 0.05 a.u.) are about 8% due to the finite number of the analyzed primary trajectories. While the quantal distribution shows two lobes, the classical one does not reproduce this quantal behavior and shows only one lobe slightly tilted towards the forward direction (in the direction of the kick). For the case of quantum distributions the lobes are related to the proper dipole transition elements and the right lobe (direction of the momentum transfer, $\mathbf{\Delta p}$) is bigger than the left lobe (opposite direction) and, in consequence, the average final momentum of the electron is positive.

Fig. 2(c) shows that SFA predicts an average momentum (center of the spot) $k_z = \Delta p = 0.5$ and is quite different from quantal and classical momentum distributions of Fig. 2(a) and (b), and therefore, ionization by a kick of $\Delta p = 0.5$ is far from the strong field regime. Since Fig. 2(c) displays the velocity distribution right after the kick (SFA), a direct comparison between Fig. 2(a) and (b) shows the strong effect of the atomic Coulomb potential on escaping electrons after the kick.

In Fig. 1(c) the energy spectrum of the electron yield ionized by a kick of strength $\Delta p = 2.5$ is displayed. In this case classical and

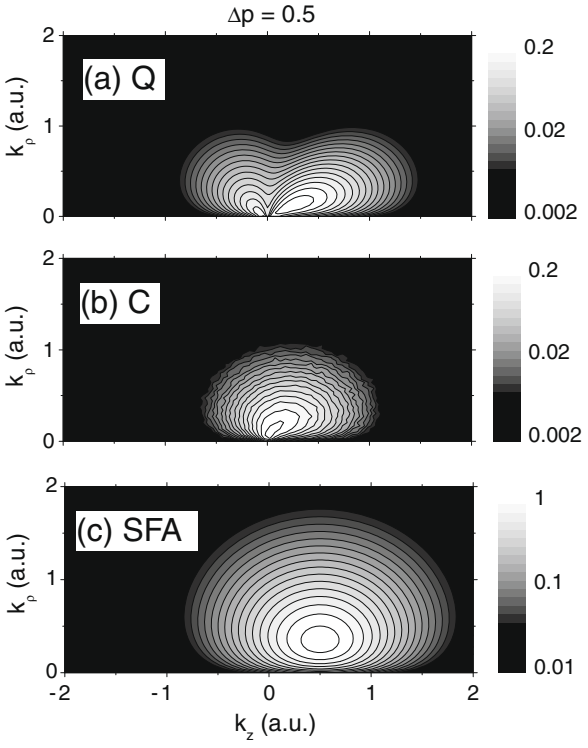

Fig. 2. Doubly-differential electron momentum distributions (logarithmic scale) in cylindrical coordinates (k_z, k_ρ). (a) Quantum, (b) classical, and (c) SFA. The momentum transfer is $\Delta p = 0.5$.

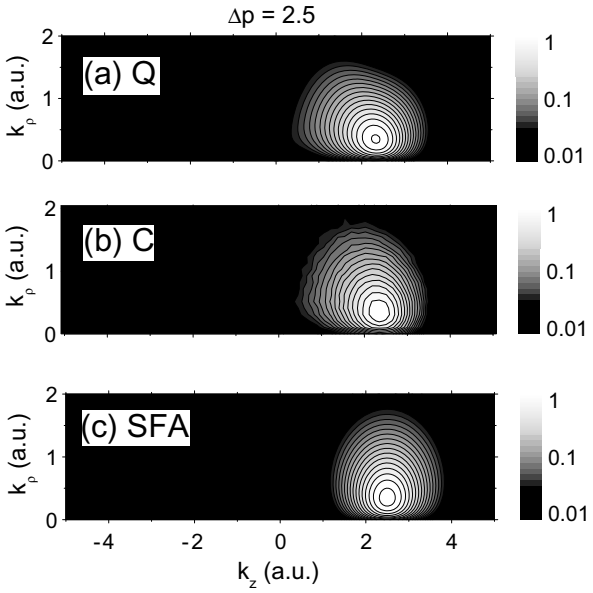

Fig. 3. Doubly-differential electron momentum distributions (logarithmic scale) in cylindrical coordinates (k_z, k_ρ). (a) Quantum, (b) classical, and (c) SFA. The momentum transfer is $\Delta p = 2.5$.

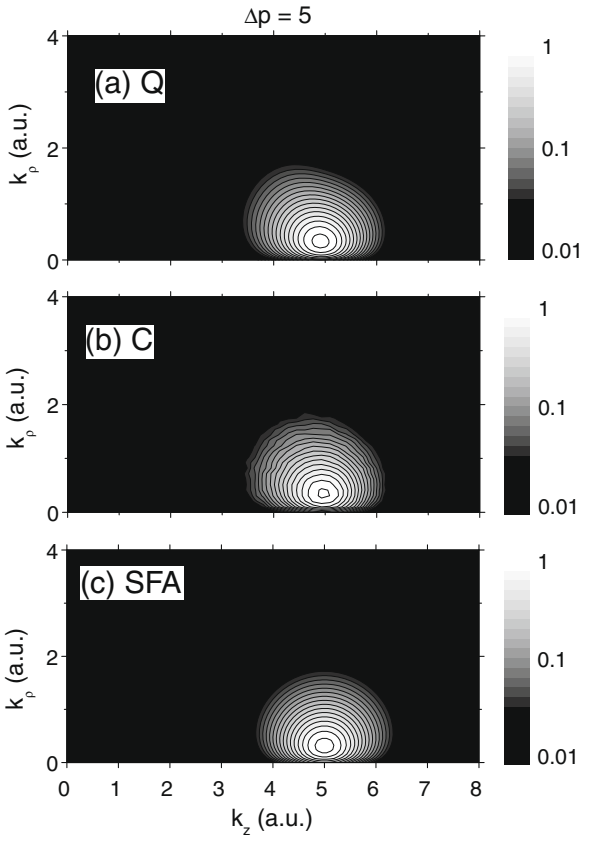

Fig. 4. Doubly-differential electron momentum distributions (logarithmic scale) in cylindrical coordinates (k_z, k_ρ). (a) Quantum, (b) classical, and (c) SFA. The momentum transfer is $\Delta p = 5$.

quantum total ionization probability are very similar 96.1% and 96.8%, respectively. Quantum–classical correspondence is observed not only in total ionization yield but also in the doubly-differential momentum distributions as displayed in Fig. 3(a) and (b). Quantum mechanics brings about only one lobe in the forward direction which can be reproduced accurately by classical mechanics. The left lobe observed for weak kicks is not present here since we are far away from the dipole regime. When compared to the SFA result of Fig. 3(c) we can essentially observe two effects: (i) the centers of the full quantum and classical distributions of Fig. 3(a) and (b) (most probable z component of the momentum) are slightly shifted towards the origin with respect to the SFA, which is exactly at $k_z = \Delta p$, and (ii) the full quantum and classical momentum distributions are weakly distorted near the origin ($\mathbf{k} = \mathbf{0}$) due to the effect of the Coulomb field. This near-threshold distortion is more evident in Fig. 1(c), where the energy distribution of the SFA drops about two orders of magnitude at $E = 0.01$ with respect to the CVA and CTMC results. This near-threshold distortion is obviously not present in the SFA momentum distribution of Fig. 3(c). We can affirm that classical distributions mimic the quantum ones even in the features that are not proper of the SFA, i.e. near-threshold structures.

For strong external fields ($\Delta p = 5$) the total ionization probability is almost 100% in both quantum and classical cases, exactly like in the SFA (Fig. 1(d)). In Fig. 4 we show that for a kick strength of $\Delta p = 5$ not only the quantum (Fig. 4(a)) and classical (Fig. 4(b)) momentum distributions are alike but the strong field regime (Fig. 4(c)) is also reached. The three doubly-differential momentum distributions look practically indistinguishable.

4. Summary

We have shown that the Coulomb–Volkov approximation (CVA) for ionization by a sudden momentum transfer describes exactly the quantum results. The velocity distribution of emitted electrons right after ionization by a sudden momentum transfer can be calculated through the strong field approximation (SFA) within both CVA and CTMC method. In this case, classical and quantum dynamics are identical. The difference between the classical and quantum final momentum distributions resides in the subsequent action of the Coulomb field.

Acknowledgements

The authors thank M.S. Gravielle for fruitful discussions on the CVA. This work was performed with financial support of CONICET and PICT 772 ANPCyT of Argentina, the Hungarian–Argentine collaboration PA05-EIII/007, the Grant "Bolyai" from the Hungarian Academy of Sciences, the Hungarian National Office for Research and Technology and the Hungarian Scientific Research Found OTKA (K72172). One of us (KT) was also partially supported by the European COST Action CM0702.

References

[1] F.H.M. Faisal, Schlegel, J. Phys. B 38 (2005) L223.
[2] D.B. Milosevic, G.G. Paulus, D. Bauer, W. Becker, J. Phys. B 39 (2006) R203.
[3] D. Bauer, D.B. Milosevic, W. Becker, J. Mod. Opt. 53 (2006) 135.
[4] D.B. Milosevic, G.G. Paulus, W. Becker, Opt. Exp. 11 (2003) 1418.
[5] P.A. Macri, J.E. Miraglia, M.S. Gravielle, J. Opt. Soc. Am. B 20 (2003) 1801.
[6] V.D. Rodriguez, E. Cormier, R. Gayet, Phys. Rev. A 69 (2004) 053402.
[7] G. Duchateau, E. Cormier, R. Gayet, Eur. Phys. J. D 11 (2000) 191;
G. Duchateau, E. Cormier, H. Bachau, R. Gayet, Phys. Rev. A 63 (2001) 053411.
[8] D.G. Arbó, J.E. Miraglia, M.S. Gravielle, K. Schiessl, E. Persson, J. Burgdörfer, Phys. Rev. A 77 (2008) 013401.
[9] R.E. Olson, C.O. Reinhold, D.R. Schultz, High-energy ion–atom collisions, in: D. Berényi, G. Hock (Eds.), Proceedings of the IVth Workshop on High-Energy Ion – Atom Collision Processes, Debrecen, Hungary, 1990, Lecture Notes in Physics 376 (1991) 69 and references therein.
[10] J.S. Cohen, J. Phys. B 18 (1985) 1759.
[11] K. Tőkési, G. Hock, Nucl. Instr. and Meth. B 86 (1994) 201.
[12] K. Tőkési, G. Hock, J. Phys. B 29 (1996) 119.
[13] L.V. Keldysh, Sov. Phys. – JETP 20 (1965) 1307;
F.H.M. Faisal, J. Phys. B 6 (1973) L89;
H.R. Reiss, Phys. Rev. A 22 (1980) 1786.
[14] D.P. Dewangan, J. Eichler, Phys. Rep. 247 (1997) 59.
[15] C.O. Reinhold, J. Burgdörfer, J. Phys. B 26 (1993) 3101;
C.O. Reinhold, M. Melles, H. Shao, J. Burgdörfer, J. Phys. B 26 (1993) L659.
[16] D.M. Volkov, Z. Phys. 94 (1935) 250.