

Chapter 1

Trajectory-Based Coulomb-Corrected Strong Field Approximation

T.-M. Yan, S.V. Popruzhenko, and D. Bauer

Abstract The strong field approximation (SFA) is one of the most successful theoretical approaches to tackle the problem of atomic or molecular ionization in intense laser fields. In the semi-classical limit, the SFA possesses an appealing interpretation in terms of interfering quantum trajectories, which mathematically originate from the saddle point approximation to the SFA transition matrix element. The trajectories not only allow to interpret particular features in photoelectron spectra in an intuitive way in terms of possible electron pathways typical for a quantum mechanical “multi-slit experiment” but also serve as a starting point for adopting Coulomb corrections.

1.1 Introduction

The development of ultrafast intense laser technology has offered the unprecedented opportunity to explore the dynamics of atomic and molecular systems. With the external light field strong enough to invoke nonperturbative multiphoton absorption and the temporal resolution of ultrafast lasers high enough to resolve the motion of electrons on the attosecond time scale, researchers are able to image electronic dynamics by means of diverse strong field processes. Among these strong field phenomena, atomic single-ionization is undoubtedly the fundamental key process and the prerequisite for the further understanding of strong field physics [1].

Experimentally, differential photoelectron momentum distributions are of essential interest because they provide a kinematically complete picture of the ionization process under study. Such measurements are possible since the invention of

T.-M. Yan · D. Bauer (✉)

Institut für Physik, Universität Rostock, 18051 Rostock, Germany

e-mail: dieter.bauer@uni-rostock.de

T.-M. Yan

Max-Planck-Institut für Kernphysik, Postfach 103980, 69029 Heidelberg, Germany

S.V. Popruzhenko

National Research Nuclear University “Moscow Engineering Physics Institute”,
Kashirskoe Shosse 31, 115409 Moscow, Russia

the so-called “reaction microscope” (COLTRIMS, cold target recoil ion momentum spectroscopy) [2].

Theoretically, the most accurate tool to explore the non-relativistic dynamics of atomic ionization is solving the corresponding time-dependent Schrödinger equation (TDSE). However, solving the TDSE for strong laser pulses in full dimensionality is prohibitive for more than two electrons. Even in the case of only one active electron, the numerical demand is very high for long wavelengths or elliptical polarization. Moreover, the result from an *ab initio* TDSE solution often lacks physical insight because the essential physics behind the appearance of particular spectral features remains hidden.

The (almost) analytical strong field approximation (SFA) [3–5] yields maximum physical insight, provided the photoelectron transition matrix element is written in terms of (interfering) quantum trajectories [1]. However, the neglect of the long-range Coulomb interaction in the ionization of neutral atoms in the SFA leads to severe discrepancies when SFA results are compared to experiment or *ab initio* numerical solutions, particularly in the low energy regime. Such disagreements include Coulomb-induced asymmetries in both elliptically [6, 7] and few-cycle linearly polarized fields [8], cusps and horn-like structures in photoelectron momentum distributions in the tunneling regime [9, 10], experimentally observed near-threshold radial structures [9, 11], and the “low-energy structure” at long wavelengths [12, 13].

Many strategies based on the SFA have been proposed in order to include Coulomb interaction, for instance a trajectory-based perturbation theory with a matching procedure for the calculation of ionization rates [14], the Coulomb–Volkov approximation (CVA) [15, 16], the eikonal-Volkov approximation (EVA) [17], the trajectory-based Coulomb-corrected strong field approximation (TCSFA) [18, 19], or the doubly distorted-wave method (DDCV) [20].

In this work, a general overview of the TCSFA is given, intending to provide an improved theoretical tool beyond the plain SFA. The introduction of the method is accompanied by a test case in which Coulomb effects are important, namely atomic hydrogen interacting with a few-cycle long-wavelength laser pulse. Interference fringes in the photoelectron spectrum are analyzed using bivariate histograms of trajectory data.

1.2 Theoretical Description of Atomic Strong Field Ionization

1.2.1 Strong Field Approximation

The idea behind the SFA is the assumption that after the electron enters the continuum at time $t = t_r$, only the interaction between the electron and the external field needs to be considered, while the influence of the binding potential is neglected. In its simplest form, the SFA accounts only for the so-called “direct” ionization, i.e., without “rescattering”. The final state of the electron characterized by the

asymptotic momentum $\mathbf{p}$ in the Keldysh–Faisal–Reiss amplitude [3–5] is a Gordon–Volkov state,

$$|\psi_{\mathbf{p}}^{(\text{GV})}(t)\rangle = e^{-iS_{\mathbf{p}}(t)}|\mathbf{p} + \mathbf{A}(t)\rangle, \quad S_{\mathbf{p}}(t) = \int^t \frac{1}{2}(\mathbf{p} + \mathbf{A}(t'))^2 dt',$$

leading to the transition matrix element [21, 22],

$$M_{\mathbf{p}}^{(0)} = -i \int_0^\infty \langle \mathbf{p} + \mathbf{A}(t') | \mathbf{r} \cdot \mathbf{E}(t) | \psi_0 \rangle e^{iS_{I_p, \mathbf{p}}(t)} dt, \quad (1)$$

with $|\psi_0\rangle$ the initial bound state of the electron, I_p the ionization potential of the atom, $\mathbf{A}(t)$ the vector potential of the light pulse, $\mathbf{E}(t) = -\partial_t \mathbf{A}(t)$ the electric field vector under the dipole approximation, and the action

$$S_{I_p, \mathbf{p}}(t) = \int^t \left[\frac{1}{2}(\mathbf{p} + \mathbf{A}(t'))^2 + I_p \right] dt'.$$

Atomic units are used unless noted otherwise.

The SFA has achieved gratifying agreement with *ab initio* results for atomic systems with a short-range potential (as is the case for electron detachment from negative ions [23]). However, the neglect of the interaction between released electrons and the long-range binding potential is shown to result in large deviations from experimental or *ab initio* results, which implies the necessity of Coulomb corrections to the SFA model.

1.2.2 Steepest Descent Method Applied to the SFA

Although the time integration in Eq. (1) can be carried out numerically with ease, the transition amplitude may be simplified using the steepest descent method [24], which is also the crucial step to implement the TCSFA. If the number of photons N of energy $\hbar\omega$ required to overcome the ionization potential I_p is large, $N = I_p/\hbar\omega \gg 1$, the time integral in the SFA matrix element is approximated by a sum over all saddle points $\{t_s^{(\alpha)}\}$,

$$M_{\mathbf{p}}^{(0)} \sim \sum_{\alpha} \frac{e^{iS_{I_p, \mathbf{p}}(t_s^{(\alpha)})}}{S''_{I_p, \mathbf{p}}(t_s^{(\alpha)})}, \quad (2)$$

where S'' denotes the second-order time derivative of S . The proportionality constant depends on I_p only [1] and is omitted here. Note that there is $S''_{I_p, \mathbf{p}}(t_s^{(\alpha)})$ in the denominator and not the square-root of it, as a modified steepest descent approach is required for the Coulomb potential [1].

The coherent summation over different trajectories which end up with the same asymptotic momentum $\mathbf{p}$ is a manifestation of the “multi-slit-in-time”-nature [27–29] of the quantum mechanical ionization process, leading to quantum interference. In addition, since $t_s^{(\alpha)}$ is complex, the calculation of trajectories has been naturally extended into the complex plane, known as the imaginary time method (ITM)

(see [30] for a review). The ITM straightforwardly includes tunneling effects. Although the SFA starts with an assumption neglecting the Coulomb interaction, the intuitive concept of quantum trajectories allows us to incorporate Coulomb effects by modifying the action integral and the trajectories accordingly.

The α th saddle point $t_s^{(\alpha)}$ satisfies the stationary phase condition or saddle-point equation (SPE)

$$\left. \frac{\partial S_{I_p, \mathbf{p}}}{\partial t} \right|_{t_s^{(\alpha)}} = 0 \quad \Rightarrow \quad \frac{1}{2} (\mathbf{p} + \mathbf{A}(t_s^{(\alpha)}))^2 = -I_p. \quad (3)$$

It is evident that, as $I_p > 0$ and $\mathbf{p}$ is real, the solution $t_s^{(\alpha)}$ is complex. Generally, smaller $\text{Im} t_s$ assign larger weights to the corresponding terms in Eq. (2). Usually, the terms with smallest $\text{Im} t_s$ have t_r near the times when the absolute value of the electric field is around a local maximum.

Expression (2), besides approximating the integral (1), also offers deeper physical insight into the ionization process by virtue of “quantum orbits” [25, 26]. At $t_s^{(\alpha)}$ a trajectory is launched, with $S_{I_p, \mathbf{p}}(t_s^{(\alpha)})$ being the corresponding action integral. The complex trajectories are a natural extension of classical trajectories which are calculated from Newton’s equation of motion, but the time propagation is along the vertical path of constant- t_r in the complex-time plane. Without Coulomb interaction the complex trajectories are

$$\mathbf{r}(t) = \int_{t_s}^t [\mathbf{A}(t') + \mathbf{p}] dt' + \mathbf{r}(t_s).$$

In order to fulfill $\text{Re} \mathbf{r}(t_s) = 0$ (the electron starts at the position of the nucleus in the origin) we require a purely imaginary $\mathbf{r}(t_s) = i \text{Im} \mathbf{r}(t_s)$ as one initial condition. The other initial condition is determined by the chosen asymptotic momentum and the solution t_s of the SPE (3),

$$\dot{\mathbf{r}}|_{t=t_s} = \mathbf{v}(t_s) = \mathbf{A}(t_s) + \mathbf{p}.$$

At time $t_r = \text{Re} t_s$ the electron reaches the classically allowed region at the “tunnel exit”

$$\begin{aligned} \mathbf{r}(t_r) = \mathbf{r}(\text{Re} t_s) &= \int_{t_s}^{t_r} [\mathbf{A}(t') + \mathbf{p}] dt' + \mathbf{r}(t_s) \\ &= -i \mathbf{p} \text{Im} t_s + \mathbf{a}(t_r) - \mathbf{a}(t_s) + i \text{Im} \mathbf{r}(t_s), \end{aligned}$$

where the excursion of a free electron in a laser field

$$\mathbf{a}(t) = \int^t \mathbf{A}(t') dt'$$

has been introduced. We can always choose the initial, purely imaginary position $i \text{Im} \mathbf{r}(t_s)$ such that $\text{Im} \mathbf{r}(t_r) = 0$. Then, the tunnel exit lies in real position space,

$$\mathbf{r}(t_r) = \text{Re} \mathbf{r}(t_r) = \mathbf{a}(t_r) - \text{Re} \mathbf{a}(t_s),$$

and for all real times $t > t_r$ the position

$$\mathbf{r}_{t \geq t_r}(t) = \int_{t_r}^t [\mathbf{A}(t') + \mathbf{p}] dt' + \mathbf{r}(t_r)$$

remains real.

1.2.3 Trajectory-Based Coulomb Correction

In this section, the key idea of the TCSFA is introduced, namely including the effect of the Coulomb potential via the modification of the quantum orbits. Henceforth, the subscript “0” is used to indicate plain SFA, “Coulomb-free” variables. The action as a function of the saddle point $t_s^{(\alpha)}$ can be recast into

$$S_{I_p, \mathbf{p}}(t_{s0}^{(\alpha)}) = C(\mathbf{p}) - \int_{t_{s0}^{(\alpha)}}^{\infty} \left[\frac{1}{2} \mathbf{v}_0^2(t) + I_p \right] dt, \quad (4)$$

where $\mathbf{v}_0(t) = \mathbf{p} + \mathbf{A}(t)$ is the velocity of an electron in the field described by $\mathbf{A}(t)$. The term $C(\mathbf{p}) = \int_0^{\infty} [\frac{1}{2} \mathbf{v}_0^2(t) + I_p] dt$ varies with different asymptotic momenta $\mathbf{p}$, but it is independent of individual saddle points $t_{s0}^{(\alpha)}$ for the same $\mathbf{p}$. Consequently, $C(\mathbf{p})$ does not contribute to the final ionization probability, since it can be factored out of the summation and eventually cancels as a phase factor.

The integrand in the second term corresponds to the Hamiltonian $H_0(t) = \frac{1}{2} \mathbf{v}_0^2(t)$ for a free electron in the electromagnetic field so that

$$S_{I_p, \mathbf{p}}(t_{s0}^{(\alpha)}) = C(\mathbf{p}) - \int_{t_{s0}^{(\alpha)}}^{\infty} [H_0(t) + I_p] dt. \quad (5)$$

When the Coulomb field is switched on, the motion of the electron is altered, i.e., $\mathbf{r}_0 \rightarrow \mathbf{r}$ and $\mathbf{v}_0 \rightarrow \mathbf{v}$, and the Hamiltonian in the action (5) is modified to include the Coulomb potential [18],

$$H_0 \rightarrow H = H_0 + U_{\text{Coulomb}} = H_0 - \frac{Z}{|\mathbf{r}(t)|}.$$

Moreover, the saddle-point times for a given *asymptotic* momentum $\mathbf{p}$ will be changed too, $t_{s0}^{(\alpha)} \rightarrow t_s^{(\alpha)}$, as the saddle-point equation (3) becomes

$$\frac{1}{2} \mathbf{v}^2(t_s^{(\alpha)}) = \frac{1}{2} (\mathbf{p}_0 + \mathbf{A}(t_s^{(\alpha)}))^2 = -I_p \quad (6)$$

because the initial canonical momentum $\mathbf{p}_0 = \mathbf{p}(t_s^{(\alpha)})$ is not conserved anymore. As a consequence, also the term $C(\mathbf{p})$ in (4) will be different for different $t_s^{(\alpha)}$ that lead to the same asymptotic momentum. In the current work, we neglect this change in $C(\mathbf{p})$.

With these modifications, we have the Coulomb-corrected transition amplitude

$$M_{\mathbf{p}}^{(0)} \sim e^{iC(\mathbf{p})} \sum_{\alpha} \frac{\exp[-i \int_{t_s^{(\alpha)}}^{\infty} (\frac{1}{2} \mathbf{v}^2(t) - \frac{Z}{|\mathbf{r}(t)|} + I_p) dt]}{S''(t_s^{(\alpha)})} \equiv e^{iC(\mathbf{p})} \sum_{\alpha} M_{\mathbf{p}}(t_s^{(\alpha)}). \quad (7)$$

In practice, the integration in (7) from $t_s^{(\alpha)}$ to infinity

$$W_{\mathbf{p}} = \int_{t_s^{(\alpha)}}^{\infty} \left(\frac{1}{2} \mathbf{v}^2(t) - \frac{Z}{|\mathbf{r}(t)|} + I_p \right) dt \quad (8)$$

is split into two parts: the sub-barrier part $W_{\mathbf{p},\text{sub}} = \int_{t_r^{(\alpha)}}^{t_s^{(\alpha)}}$ and the real-time propagation part $W_{\mathbf{p},\text{re}} = \int_{t_r^{(\alpha)}}^{\infty}$.

1.2.4 Applications and Numerical Implementation

Because of the azimuthal symmetry about the polarization axis of a linearly polarized laser field in dipole approximation, it is sufficient to consider a 2D momentum plane $\mathbf{p} = (p_z, p_x)$ where $p_z = p_{\parallel}$ is in the polarization direction and $p_x = p_{\perp}$ is in any perpendicular direction.

The steps to evaluate the transition matrix element of atomic ionization are:

- (i) Given $\mathbf{p}_0$ and $t_{\text{guess}}^{(\alpha)}$, solve the SPE (6) with a complex root-finding method to obtain the saddle point $t_s^{(\alpha)}$. For the value of $t_{\text{guess}}^{(\alpha)}$, one may choose the corresponding plain-SFA value.
- (ii) Calculate the sub-barrier action $W_{\mathbf{p},\text{sub}}$. The current work neglects the sub-barrier Coulomb correction. Hence, $W_{\mathbf{p},\text{sub}}$ can be calculated analytically, as in plain (quantum orbit) SFA.
- (iii) Solve the ordinary differential equations of motion in real position space

$$\dot{\mathbf{r}}(t) = \mathbf{p}(t) + \mathbf{A}(t), \quad (9)$$

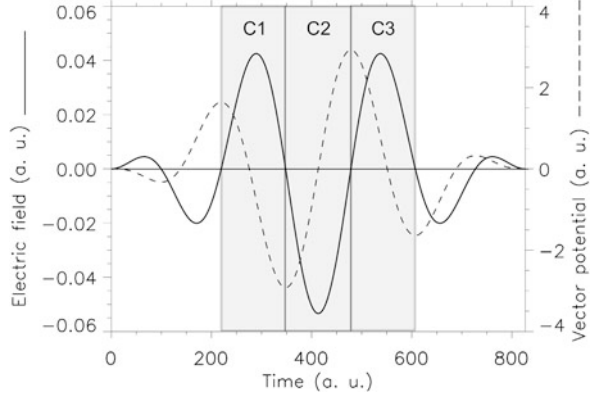
$$\dot{\mathbf{p}}(t) = -\frac{Z\mathbf{r}(t)}{|\mathbf{r}(t)|^3} \quad (10)$$

for real times $t > t_r$ until the laser is switched-off at time T_p . The initial conditions are

$$\mathbf{r}(t_r) = \text{Re } \mathbf{r}(t_r) = \mathbf{a}(t_r) - \text{Re } \mathbf{a}(t_s), \quad \mathbf{p}(t_r) = \mathbf{p}_0. \quad (11)$$

- (iv) Calculate $W_{\mathbf{p},\text{re}}$ along the trajectory $\mathbf{r}$ for the real time propagation. Steps (iii) and (iv) can be performed simultaneously.
- (v) After the laser is switched off at T_p the asymptotic momentum $\mathbf{p}$ can be found employing Kepler's formulas [11].
- (vi) Calculate the individual transition amplitude $M_{\mathbf{p}}(t_s^{(\alpha)})$ in Eq. (7) for this trajectory.

Fig. 1.1 The $\sin^2$ vector potential and the electric field, $\omega = 0.0228$ (wavelength $2 \mu\text{m}$), $E_0 = 0.0534$ (intensity $1 \times 10^{14} \text{ W/cm}^2$) and $N_c = 3$. To facilitate the analysis of the electron emission times, we indicate three time intervals C1–C3



If the laser pulse covers several cycles, each choice of $\mathbf{p}_0$ generally leads to several saddle-points and thus to several trajectories. However, since only the saddle points with the lowest imaginary parts possess the largest weights, in practical calculations only a few trajectories need to be taken into account for each $\mathbf{p}_0$.

While the trajectory-based calculation is conceptually simple, a large data set of trajectories is required to obtain smooth spectra with good statistics. Fortunately, the method is trivial to parallelize because of the independence of the trajectories. In practice, we launch trajectories with random, uniformly sampled $\mathbf{p}_0$. For each trajectory, one obtains the asymptotic momentum $\mathbf{p}$ and the individual transition matrix element $M_{\mathbf{p}}(t_s^{(\alpha)})$ using the recipe above. All information related to this trajectory can be stored for further analysis.

With all trajectories available, one can calculate the momentum distribution of the ionization probability on a grid representing the final momentum $\tilde{\mathbf{p}}$. To that end trajectories are binned according to their asymptotic momentum $\mathbf{p}$, and the total transition amplitude for momentum $M_{\tilde{\mathbf{p}}}$ is the sum over all transition amplitudes $M_{\mathbf{p}}^{(i)}$, $M_{\tilde{\mathbf{p}}} = \sum_i M_{\mathbf{p}}^{(i)}$. Here, the trajectory whose corresponding transition amplitude is $M_{\mathbf{p}}^{(i)}$ should have its asymptotic momentum $\mathbf{p}$ in the bin centered at $\tilde{\mathbf{p}}$, and i represents the index of trajectories satisfying this condition.

1.3 Results and Discussion

In order to demonstrate the usefulness of the TCSFA method as a tool for a detailed analysis of photoelectron spectra, we consider the test case of atomic hydrogen ($I_p = 0.5$) in a linearly polarized (along the z -axis in the $(p_z p_x)$ -plane) light field described by the vector potential

$$A(t) = -\frac{E_0}{\omega} \sin^2\left(\frac{\omega t}{2N_c}\right) \sin \omega t, \quad (12)$$

where ω is the laser frequency, E_0 is the peak electric field strength, and N_c is the number of optical cycles. The parameters are listed in the caption of Fig. 1.1.

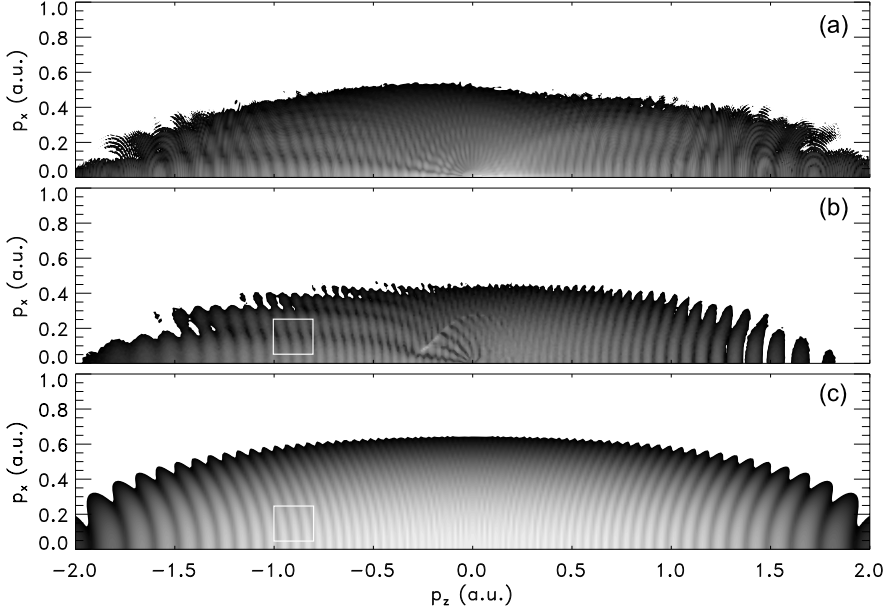


Fig. 1.2 Logarithmically scaled photoelectron momentum distributions in the (p_z, p_x) -plane ($p_{\parallel} = p_z$) calculated using (a) TDSE, (b) TCSFA, and (c) SFA. Each spectrum was normalized to its maximum value, with orders of magnitudes 4, 4.4 and 2, respectively, for the convenience of comparison. The white box-frames in (b) and (c) indicate the zoomed regions to be studied

Figure 1.2 shows the photo-electron momentum distributions calculated with different methods: the TDSE [31], the TCSFA and the plain SFA. The TDSE result serves as a benchmark to check the validity of other methods. Several important spectral features are observed. Firstly, the momentum spectrum exhibits a globally asymmetrical distribution along the z -direction due to the few cycles in the laser pulse [32]. In addition, the distribution reveals a near-threshold ($\mathbf{p} \simeq 0$) spoke-like pattern [11]. At higher energies side-lobes are visible for $p_z < 0$, which have been shown to originate from the intra-cycle interference of quantum trajectories [33]. All these Coulomb effects are well reproduced by the TCSFA calculation, while lacking in the plain SFA result Fig. 1.2(c). If the conversion from the momentum distribution to the energy spectra is made, the caustic with the semi-classical calculation in Fig. 1.2(b) is shown to form the reported spike-like peak in mid-infrared fields, known as the low-energy structure (LES) [12, 13, 19, 34, 35].

1.3.1 Categorization of Trajectories and Partial Reconstruction

The origin of the difference between the excellent TCSFA result in Fig. 1.2(b) and the poor plain-SFA result in Fig. 1.2(c) can now be traced back to the modification

Table 1.1 Categorization of the trajectories in the TCSFA

Types	Longitudinal condition	Transversal condition
T1	$p_z(\infty)z(t_r) > 0$	$p_x(t_r)p_x(\infty) > 0$
T2	$p_z(\infty)z(t_r) < 0$	$p_x(t_r)p_x(\infty) > 0$
T3	$p_z(\infty)z(t_r) < 0$	$p_x(t_r)p_x(\infty) < 0$
T4	$p_z(\infty)z(t_r) > 0$	$p_x(t_r)p_x(\infty) < 0$

of quantum orbits because of the Coulomb potential acting on the emitted electron. Two types of trajectories are known in plain SFA, commonly called “short” and “long” [36]. In the following we label these trajectories T1 and T2, respectively. However, two additional types of trajectories, T3 and T4, need to be introduced when long-range Coulomb interaction is included [19]. The definitions of the trajectory types 1–4 are listed in Table 1.1. The short trajectories T1 start at a tunnel exit that points already towards the detector, with the initial transversal canonical momentum and the asymptotic one having the same sign. In other words, the electron flies from the beginning on “into the right direction”. The long trajectories T2 instead start in the “wrong” direction but already with the “right” sign of the transversal canonical momentum. In plain SFA, the canonical momentum is conserved so that there is no other way for the electron than having the “right” asymptotic canonical momentum from the very beginning. With Coulomb attraction at work, however, the lateral momentum may be reversed, leading to trajectories T3, not present in plain SFA. Finally, trajectories of type T4 start off in the “right” direction with respect to the laser polarization direction but with a transversal canonical momentum that changes sign during the propagation towards the detector.

With the above categorization as a natural extension of the quantum orbits in the plain SFA, “partial spectra” can be reconstructed using only partial type(s) of trajectories. It is possible to infer the role of trajectories which satisfy certain conditions by comparing their partial spectra with the full spectra. Momentum spectra constructed from individual types of trajectories are shown in Fig. 1.3. For T1, a ring-like distribution because of significant interference is visible in the negative-half momentum plane $p_z < 0$ while a structureless distribution emerges in the positive-half plane. The interference in the negative-half plane originates from the coherent superposition of trajectories whose t_r fall into the time interval C1 and C3 (as indicated in Fig. 1.1). Since $E(t)$ in C1 and C3 are the same in magnitude, the weights for trajectories born in these intervals are similar, leading to significant inter-cycle interferences. Instead, in the positive-half plane, since the tunneling probability depends exponentially on the field strength, the ionization is mainly confined to trajectories born within the time interval C2 around the main peak of $E(t)$. The weights of these trajectories are typically larger than those from the side-peaks. Thus, hardly can any clear interference develop. Similarly, the explanation also applies to the partial spectra of T2. However, since T2 represents the “long” trajectory with the initial “tunnel exit” $z(t_r)$ opposite to that of T1, the spectrum is reversed with respect to p_z .

For the trajectory-types T1 and T2, the transversal momentum does not change its sign, and the Coulomb-corrections are rather small, as can be seen by comparison

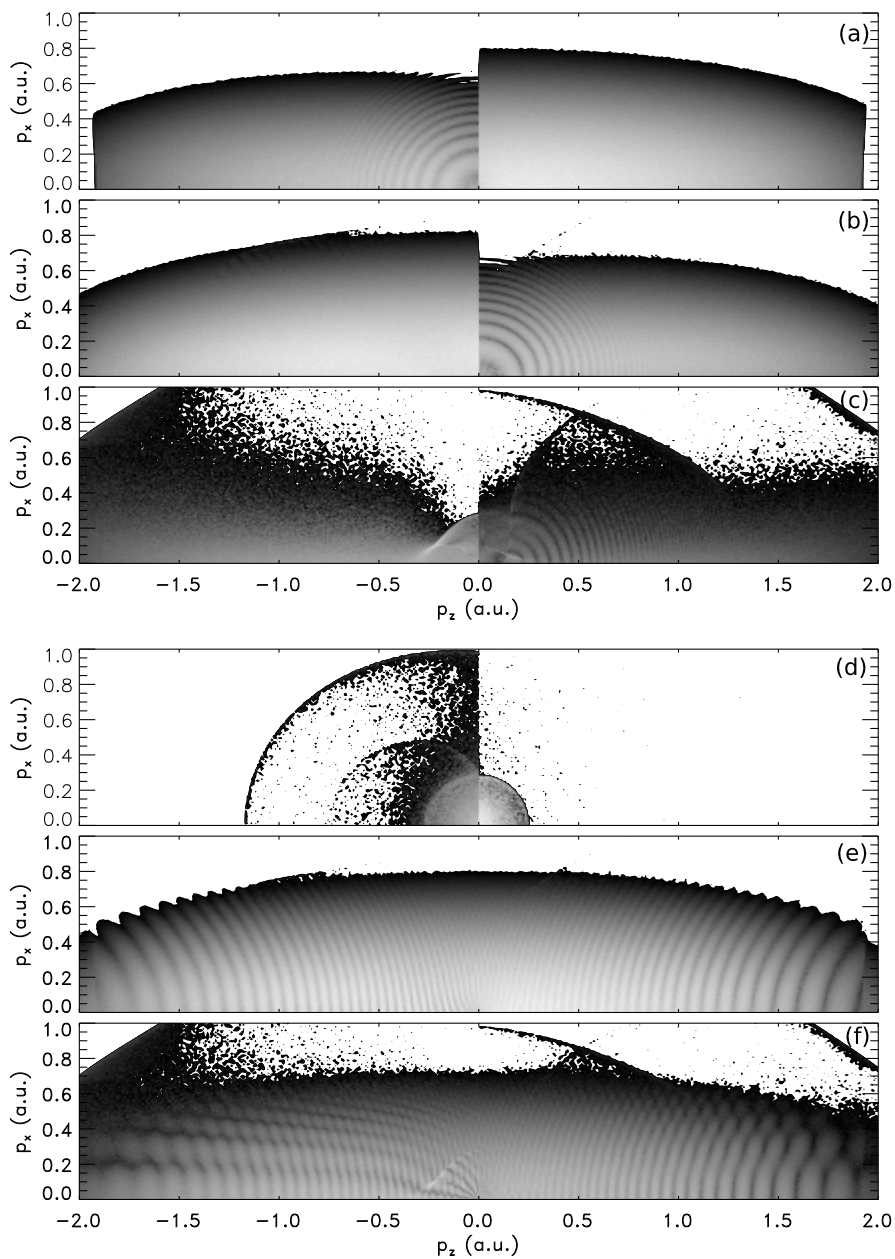


Fig. 1.3 Partial distributions constructed from different types of trajectories: (a) T1, (b) T2, (c) T3, (d) T4, (e) T1 + T2 and (f) T1 + T2 + T3

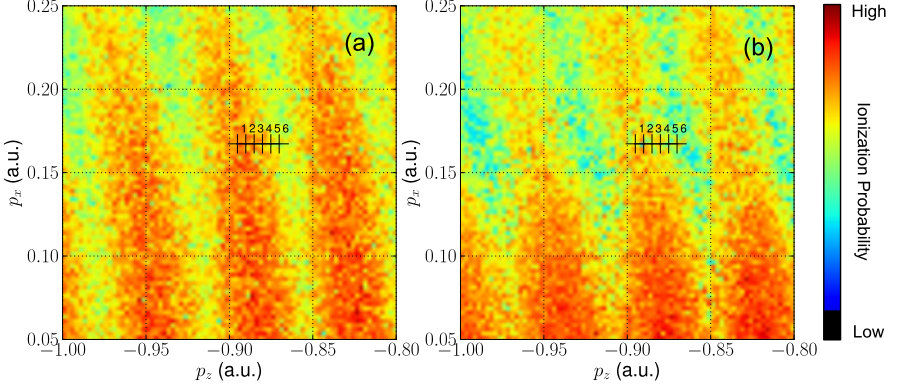


Fig. 1.4 Zoom into spectra of Fig. 1.2(c) and Fig. 1.2(b), where the *white box-frames* indicate the zoomed regions, for the SFA (a) and the TCSFA (b). At selected points, shown by *crosses* ($p_z \in [-0.9, -0.87]$, $p_x = 0.17$) and labeled 1–6, the relation between constructive or destructive interference and quantum trajectories will be illustrated below

between the SFA result in Fig. 1.2(c) and the spectra for T1 + T2 in Fig. 1.3(e). Because the Coulomb-corrected T1 and T2 alone do not yield the correct spectrum, T3 and T4—not existent in plain SFA—are obviously important. In fact, good agreement is achieved when trajectories of type T3 are included, as is shown in Fig. 1.3(f). Trajectories T3 change the sign of the transversal momentum while moving from the tunnel exit to the detector. This is only possible because of a rather strong interaction with the Coulomb field. It results in some striking features, as is shown in Fig. 1.3(c): (i) The weights of trajectories T3 are sufficiently large, comparable to those of T1 or T2, to form the side-lobes. Exaggerated local maxima, known as caustics, are also visible. In Fig. 1.3(c), a caustic is located at $\mathbf{p} = (-0.2, 0.1)$, related to the recently discovered LES [12, 13], as discussed in [19].

1.3.2 Statistical Trajectory-Based Analysis

The partial spectra can be used for a global analysis, but sometimes one is more interested in the origin of certain spectral features, for instance interference fringes.

Figure 1.4 presents a zoom into Figs. 1.2(b, c) with sampling points 1–6 indicated. The points connect an interference peak with the right-neighboring interference dip caused by intra-cycle interference. Since the TCSFA is equivalent to the SFA when $Z = 0$, the SFA has been also implemented with the trajectory-based method. The selected points reside in the valley between two side-lobes in the TCSFA result Fig. 1.2(b).

Figures 1.5(a–f) show the individual trajectories' $M_{\mathbf{p}}$ in the complex plane that contribute to the spectrum $\Delta p = 0.005$ around the sampling points 1–6 in Fig. 1.4(a). Each plot has two arcs defined as A1 and A2. The points in the origin represent $M_{\mathbf{p}}$ with negligibly small norms. As we move from sampling point

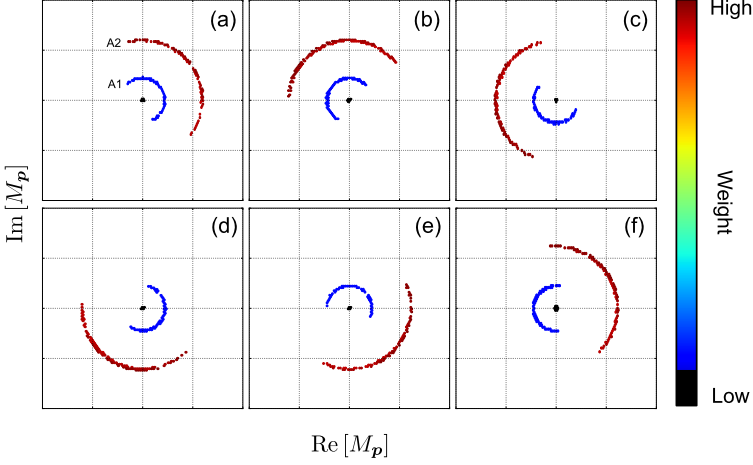


Fig. 1.5 Bivariate histograms of $M_{\mathbf{p}}$ in the complex plane for the SFA. The plots (a)–(f) may be viewed as “phase diagrams” for the points 1–6 in Fig. 1.4(a). The final-momentum bin in the (p_z, p_x) -plane for each of the points had a radius $\Delta p = 0.005$. Each of the points $M_{\mathbf{p}}$ with similar norms $|M_{\mathbf{p}}|$ construct arcs. In each panel two arcs [labeled by A1 and A2 in (a)] are visible. The color represents the weight of the $M_{\mathbf{p}}$ -distribution in hexagonal bins (the weight is defined as $\sum_{\alpha=1}^{n_i} |M_{\mathbf{p}}^{(i,\alpha)}|$ with n_i the number of trajectories in the i th bin and $|M_{\mathbf{p}}^{(i,\alpha)}|$ the norm of the α th $M_{\mathbf{p}}$)

1 to point 6 in Fig. 1.4(a), the two arcs rotate counter-clockwise at different rates, which leads to a change in the phase difference between them. The $\mathbf{p}$ -dependent phase difference in the doubly-differential momentum spectra forms the interference pattern: when A1 and A2 align in the same direction, as shown in Fig. 1.5(a), the condition for constructive interference is satisfied to form the maximum in the spectrum. The opposite alignment of A1 and A2, as shown in Fig. 1.5(f), leads to destructive interference and a minimum.

When we apply the same analysis to the TCSFA, as shown in Fig. 1.6, one more arc than for the SFA-case is observed. Indeed, the outermost arc A3 belongs to the new trajectory-type T3 because of the Coulomb potential. The inner two arcs are the counterparts of the two arcs present in the plain-SFA result Fig. 1.5. They only differ by a phase shift due to Coulomb interaction. Similar to the phase diagram for the SFA, the arcs A1 and A2 rotate at different rates, which forms the vertically aligned interference fringes. However, because of A3, which aligns opposite to A2 while rotating at a similar rate, the net contribution of trajectories associated with A2 is reduced. This destructive interference results in a side-lobe minimum clearly visible in the center of the white box in Fig. 1.2(b).

The statistical analysis in the complex $M_{\mathbf{p}}$ -plane provides direct evidence that the trajectories of A3 play the essential role in building up the side-lobes. The comparison of SFA and TCSFA results allows to quantify relative phase shifts because of Coulomb interaction.

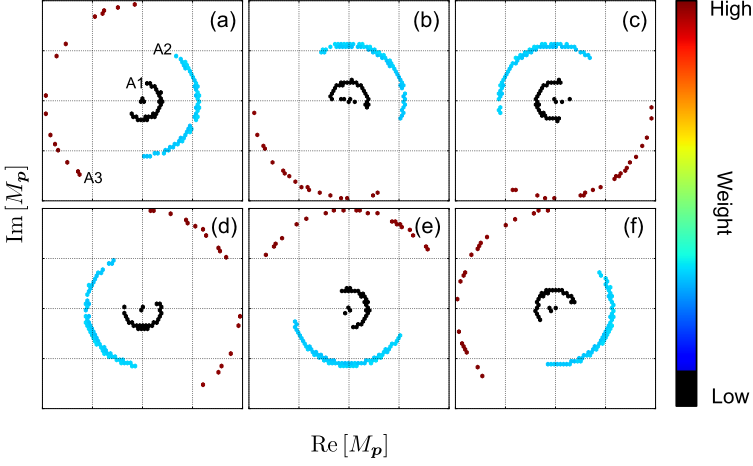


Fig. 1.6 Same as Fig. 1.5 but for the TCSFA

By mapping the individual transition amplitudes to other trajectory-related quantities a detailed insight in any spectral feature may be gained. Figure 1.7 gives an example for the first sampling point in 1.4(b). Figure 1.7(a) maps the arcs in the complex M_p -plane to the trajectory-type, showing that A1 consists of T1, A2 of T2, and A3 of T3 trajectories. The trajectories T4 map into a dot at the origin in the complex M_p -plane due to their negligibly small weights. Figure 1.7(b) together with the knowledge from (a) shows that the T1 trajectories originate from a tunnel exit at $z(t_r) \simeq -11$ while T2 and T3 start both from the opposite side at $z(t_r) \simeq 10$. From the remaining two panels in Fig. 1.7 we infer, e.g., that T3 trajectories are born close to the peak of the electric field [see Fig. 1.7(c)] within the time interval C1 of Fig. 1.1, with the smallest imaginary part of the saddle-point time [see Fig. 1.7(d)].

Figure 1.8 visualizes the trajectories for sampling point 1 in Fig. 1.4 for both TCSFA and SFA. Trajectories T1 are directly driven from the tunnel exit to the detector, and the Coulomb field does not influence T1 substantially. T2-trajectories are slightly influenced by the Coulomb attraction while T3-orbits owe their mere existence to the Coulomb potential. Only with the Coulomb potential present is it possible to reverse the lateral momentum.

1.4 Conclusion

The momentum distributions of photoelectrons after strong-field ionization exhibit rich structures, even for the simplest system of atomic hydrogen in a linearly polarized field. To understand the ionization dynamics that leads to particular spectral features, the quantum orbit-based TCSFA method has been introduced. Coulomb interaction between the outgoing electron and the residual ion is taken into account by

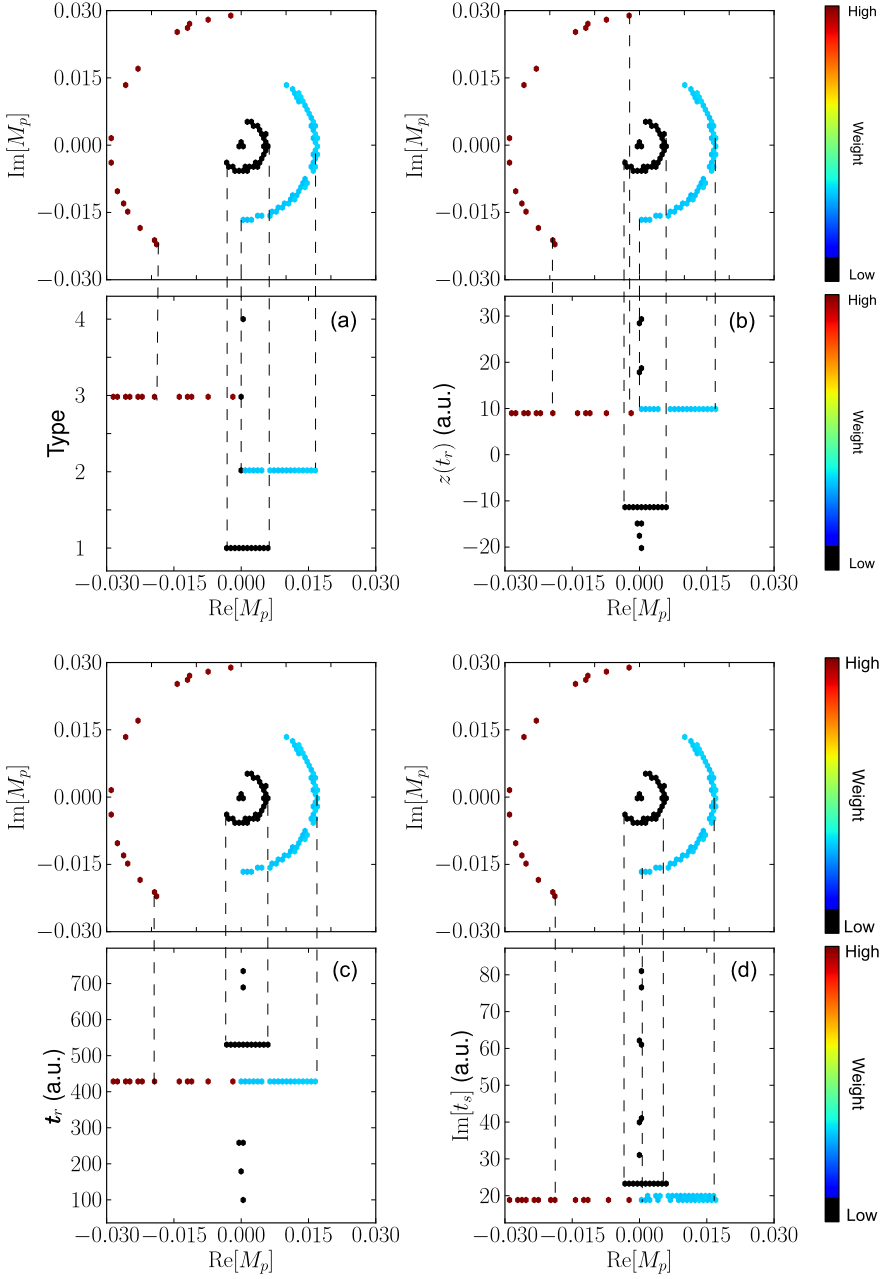
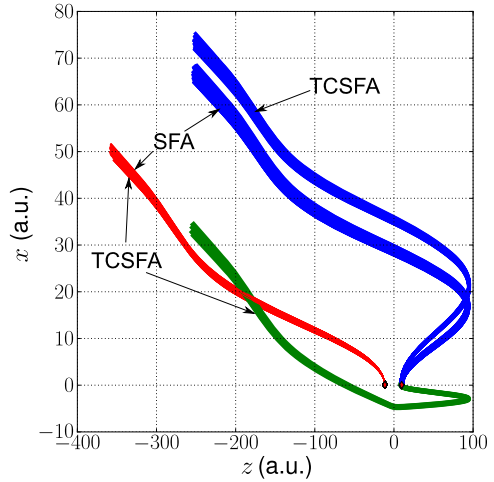


Fig. 1.7 Further analysis of Fig. 1.6(a). Mapping from the complex M_p -plane to the trajectory type (a), tunnel exit (b), emission time t_r (c), and imaginary part of the saddle-point time (d)

Fig. 1.8 Trajectories associated with the sampling point 1 for both the TCSFA and the plain SFA: T1 (red), T2 (blue) and T3 (green, exists only in TCSFA). Trajectories T2 and T3 are born within the time interval C2 at positive z , while T1 is born within C1 with the tunnel exit located at negative z



modifying the plain-SFA quantum orbits accordingly. The 2 μm case study demonstrated good agreement of TCSFA results and *ab initio* TDSE calculations. Because of the semi-classical condition $I_p/\hbar\omega \gg 1$ the TCSFA yields less satisfactory results for shorter wavelengths.

Coulomb effects influence the left-right asymmetry in photoelectron spectra, they modify the interference structure, leading, e.g., to side-lobes, and they create LESs. The analysis of trajectories in the TCSFA shows that the Coulomb interaction introduces new types of trajectories which may modify both the interference pattern (leading, e.g., to side-lobes) and the number of orbits ending up in a final momentum bin (leading, e.g., to the LES). Recent work has been devoted to the Coulomb-correction of the sub-barrier electron dynamics [37].

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