The ionization of atoms by strong, low-frequency fields can generally be described well by assuming that the photoelectron is, after the ionization step, completely at the mercy of the laser field. However, certain phenomena, like the recent discovery of low-energy structures in the long-wavelength regime, require the inclusion of the Coulomb interaction with the ion once the electron is in the continuum. We explore the first-principles inclusion of this interaction, known as analytical $R$-matrix theory, and its consequences on the corresponding quantum orbits. We show that the trajectory must have an imaginary component, and that this causes branch cuts in the complex time plane when the real trajectory revisits the neighbourhood of the ionic core. We provide a framework for consistently navigating these branch cuts based on closest-approach times, which satisfy the equation $r(t) \cdot v(t) = 0$ in the complex plane. We explore the geometry of these roots and describe the geometrical structures underlying the emergence of LES in both the classical and quantum domains.

The interaction of atoms and molecules with intense lasers is a rich field, and provides challenges for theory to describe non-perturbative phenomena which often bridge a large range of energy scales. A recent example of this is the discovery of low-energy structures (LES) [1, 2] in photoionization by strong, long-wavelength fields where, in addition to above-threshold electrons that absorb many more photons than required to reach the continuum, a strong peak is observed at energies far below the mean oscillation energy of electrons in the field.

This was unexpected [3], as the strong-field approximation (SFA) [4] typically predicts a smooth, featureless spectrum at low energies, and SFA is generally expected to improve in accuracy as the frequency decreases and the system goes deeper into the optical tunnelling regime. This triggered active interest in developing theoretical methods to describe the LES, and in identifying the physical mechanisms that create them.

Numerical simulations of the time-dependent Schrödinger equation (TDSE) do reproduce the structure [1], though they are particularly demanding at long wavelengths. Simulations done with and without the ion’s long-range Coulomb potential [5, 6] indicate that its role is essential in producing the LES. Similarly, Monte Carlo simulations [6–9] using classical trajectories involving both the laser and the Coulomb field support this conclusion.

From a semiclassical perspective, it is indeed possible to include the effect of the ion’s potential when the electron is already in the continuum. This can be done via a perturbative Born series, like those used to explain high-order ionization [10]; here the LES emerges as electrons that forward-scatter once at the ion [11–14]. Alternatively, the SFA can be reformulated to include the effect of the Coulomb field on the underlying trajectories [15–17]; the resulting Coulomb-corrected SFA (CCSFA) also points to forward-scattered electrons [18]. First-principles analytical methods to include the Coulomb field’s effect on the wavefunction’s phase, known as analytical $R$-matrix theory (ARM) [19–24], are as yet untested in this regime. Analysis of the classical trajectories involved in the scattering points more specifically at soft recollisions, where the electron does not hit the core head-on, but is instead softly deflected as it approaches the ion with nearly zero velocity, near a turning point of the laser-driven trajectory [25, 26]. Although these trajectories spend enough time near the ion that the effect of its potential is no longer perturbative (and can in fact cause chaotic dynamics [27]), a comparison of the different models suggests that the LES are rooted in the pure laser-driven orbits of the simple-man’s model, and that the role of the Coulomb potential is to enhance their contribution [28].

This raises an intriguing possibility, because there is in general a discrete sequence of soft-recolliding trajectories [26, 28], shown in Fig. 1, which spend increasing amounts of time in the continuum before recolliding, and which should appear as distinct peaks in photoelectron spectra. In this work we extend this sequence and show that there are, in fact, two families of soft-recolliding trajectories, which revisit the ion at even or odd numbers of half-periods after ionization.

FIG. 1. Trajectories with soft recollisions after tunnel ionization, for a Keldysh parameter of $\gamma = 0.75$. 
The previously-described trajectories [26, 28–30] recollide after an odd number of half-periods, and their drift energy is a constant multiple of the ponderomotive potential $U_p$. In contrast, trajectories with soft recollisions at integral multiples of the laser period have lower energies, of around 1 meV for common experimental parameters, which scale rather unfavourably as $1/U_p$. This series seems to have been overlooked, but the low energies mean that the peaks can (and, in fact, will) contribute to the ‘zero-energy structure’ (ZES) found recently [31–33]. Moreover, we show that both families of soft recollisions come up naturally within the analytical $R$-matrix theory of photoionization [19–24]. The ARM theory implements the intuition that the dominant effect of the ion’s electrostatic potential on the photoelectron is a phase, and makes this intuition rigorous via the use of eikonal-Volkov wavefunctions [34, 35] for the photoelectron. As in SFA treatments, this results in a time integral over the ionization time which, when approximated using saddle-point methods, produces a quantum-orbit picture based on semiclassical trajectories.

This first-principles approach has the advantage that it provides initial conditions for the trajectories by matching the eikonal-Volkov solution away from the core to the bound wavefunction near the core, using the WKB approximation for the bound wavefunction. In particular, the trajectories produced by this matching procedure are real-valued at the entrance to the classically-forbidden region, and this results in a nonzero imaginary position at real times, after exiting the classically-forbidden region. Thus, ARM operates with quantum orbits [36] which, in contrast to their purely real-valued counterparts in the Coulomb-corrected SFA [15–18], can change the amplitude of their contribution after ionization, i.e., after the tunnelling electron leaves the classically forbidden region [22, 23]. Mathematically, this change in the amplitude comes through the imaginary part of the position, which results in an imaginary part of the action that directly affects the amplitude. Physically, this mirrors the dynamical focusing effect found in approaches that use the full classical trajectory [25, 26].

The importance and the effect of the imaginary part of the semiclassical trajectory is most strongly felt when the electron revisits the core. Mathematically, one needs to extend the core potential into the complex plane. When the real part of the trajectory is small, this analytical continuation has a branch cut which cannot be integrated across. This branch cut must be managed carefully, as it can preclude several standard choices of integration contour, including in particular the contour going from the ionization time directly to the real time axis and then along it. In these cases, one needs a more flexible approach towards contour choice; to ease this choice we briefly describe user-friendly software [37, 38] to visualize the effects on the complex-valued position of different contour choices.

Moreover, we present a method for consistently and programmatically navigating the Coulomb branch cuts to calculate photoelectron spectra. This method is based on the fact that the branch cuts come in pairs which always contain between them a saddle point of the semiclassical distance to the origin, $\sqrt{r(t)^2}$; this saddle point is a solution to the closest-approach equation $r(t) \cdot v(t) = 0$ on the complex plane. These times of closest approach offer a rich geometry of their own, both with complex quantum orbits and within the more restricted simple man’s model. More practically, by choosing appropriate sequences of closest-approach times, one can systematically choose correct integration contours.

Within this framework, soft recollisions appear as complex interactions between different sets of branch cuts, marked by close approaches between two or three closest-approach saddle points and by topological changes in the branch cut configuration. This happens only at very low transverse momenta, and is managed well by our method. Nevertheless, the increased time spent by the electron near the ion – mirrored in the ARM formalism by close approaches between singularities and saddle points – results in an increase in the amplitude that reflects the photoelectron peaks seen in experiments.

In the current approach, the Coulomb field of the ion is allowed to influence the phase of the wavefunction (and from there the ionization amplitude), but not the underlying trajectory. A first-principles approach based on the full trajectory is still lacking, but such a theory will likely require the trajectory to be real before it enters the classically-forbidden region during the ionization step. It is then likely that such a theory will contain many of the elements we describe for the laser-driven trajectories, including the branch cut behaviour and its navigation. In that sense, our work is a roadmap for those difficulties and their resolution.

This paper is structured as follows. In Section I we explore soft recollisions for the classical trajectories of the simple man’s model, giving simple approximations for the momenta that produce them, and we explore their scaling. In Section II we derive a simple version of ARM theory, emphasizing the features that give rise to complex-valued positions for the quantum orbits.

We then examine, in Section III, the ways in which complex-valued positions give rise to branch cuts and the cases in which the latter make more sophisticated contour choices necessary. In Section IV we study the geometry of the times of closest approach, both within the simple man’s model and for the ARM quantum-orbit picture, and explain their use for navigating integration contours around the Coulomb branch cuts. We then present the resulting photoelectron spectra in Section V and summarize our results in Section VI. In addition, we provide supplementary information [39] with interactive 3D versions of several figures in this paper.

I. SOFT RECOLLISIONS IN CLASSICAL TRAJECTORIES

The simplest approach to the dynamics of a photoelectron after tunnel ionization is known as the simple man’s model. In its quantum version it accounts for the tunnelling process using the strong-field approximation, and then allows the electron to follow a laser-driven trajectory after it exits the tunnelling barrier. Within the SFA, the electron has velocity

$$v(t) = p + A(t)$$  \hspace{1cm} (1)
where \( \mathbf{p} \) is the canonical momentum registered at the detector. The electron is ‘born’ into the continuum at the origin at a complex starting time \( t_s = t_0 + i\tau_T \) which obeys

\[
\frac{1}{2} (\mathbf{p} + \mathbf{A}(t_s))^2 + I_p = 0, \tag{2}
\]

where \( \mathbf{A}(t_s) = -\int_0^{t_s} \mathbf{F}(t)dt, \mathbf{F}(t) = F \cos(\omega t) \mathbf{z} \) is the laser’s electric field, we take to be a monochromatic, linearly polarized pulse, and \( I_p = \frac{1}{2} n^2 \) is the ionization potential. (We use atomic units unless otherwise noted.) The resulting trajectory is then

\[
r_{cl}(t) = \int_{t_s}^t (\mathbf{p} + \mathbf{A}(\tau)) \, d\tau, \tag{3}
\]

which is in general complex-valued.

Throughout this work, we understand a ‘soft recollision’ to mean a trajectory which has a laser-driven turning point, with essentially zero velocity, in the neighbourhood of the ion [25, 26]. This can occur for a range of impact parameters, and the most relevant trajectories will pass within a few bohrs of the ion. However, it is often easier to identify those laser-driven trajectories that ‘go through’ the ionic core, so we focus on them in the understanding that the neighbouring trajectories are the most relevant.

Thus, to look for soft recollisions in the corresponding classical trajectories, we require that the real parts of both the velocity and the position vanish:

\[
\begin{cases}
\text{Re} [z_{cl}(t_r)] = \text{Re} \left[ \int_{t_s}^{t_r} (p_z + A(\tau)) \, d\tau \right] = 0 & \text{(4a)} \\
z_z(t_r) = p_z + A(t_r) = 0. & \text{(4b)}
\end{cases}
\]

This can be expressed as

\[
\begin{cases}
z_{\text{exit}} + p_z(t_r - t_0) + \frac{F}{\omega^2} \left( \cos(\omega t_r) - \cos(\omega t_0) \right) = 0 & \text{(5a)} \\
p_z = \frac{F}{\omega} \sin(\omega t_r) = 0, & \text{(5b)}
\end{cases}
\]

where

\[
\begin{align*}
z_{\text{exit}} &= \text{Re} \left[ \int_{t_s}^{t_0} (p + A(\tau)) \, d\tau \right] \\
&= \frac{F}{\omega^2} \cos(\omega t_0) (1 - \cosh(\omega \tau_T)) \tag{6}
\end{align*}
\]

is known as the tunnel exit.

This system can be solved numerically, but it is more instructive to consider its linearized version with respect to \( p_z \), since all the soft recollisions happen at small energies with respect to \( U_p \). To do this we express the starting time as

\[
t_0 + i\tau_T = t_s = \frac{1}{\omega} \arcsin \left( \frac{\omega}{F} p_z + ik \right) \\
\approx \frac{p_z}{F} \left( \frac{1}{\sqrt{1 + \gamma^2}} + i \frac{\gamma}{\omega} \right) \arcsinh (\gamma), \tag{7}
\]

where \( \gamma = \omega k / F \) is the Keldysh parameter, so that

\[
z_{\text{exit}} \approx - \frac{F}{\omega^2} \left( \sqrt{1 + \gamma^2} - 1 \right). \tag{8}
\]

In the tunnelling limit of \( \gamma \ll 1 \), \( z_{\text{exit}} \) reduces to \(-I_p/F\) as expected.

The linearized system now reads

\[
\begin{cases}
p_z(t_r) + \frac{F}{\omega^2} \left( \cos(\omega t_r) - \sqrt{1 + \gamma^2} \right) = 0 \tag{9a} \\
p_z = \frac{F}{\omega} \sin(\omega t_r) = 0, \tag{9b}
\end{cases}
\]

and to obtain a solution we must linearize \( t_s \) with respect to \( p_z \). Examination of the numerical solutions of the original system shows that soft recollisions exist for every half period after \( \omega t_r = 2\pi \), so we write

\[
\omega t_r = (n + 1)\pi + \omega \delta t_r \tag{10}
\]

with \( n = 1, 2, 3 \ldots \) indexing the solutions. With this we obtain from (9b) that \( \delta t_r \approx (-1)^{n+1} p_z/F \) and \( \cos(\omega t_r) \approx (-1)^{n+1} \). This gives in turn the drift momentum of the successive soft-recolliding trajectories as

\[
p_z^{sr} \approx \frac{F}{\omega} \frac{\sqrt{1 + \gamma^2} + (-1)^n}{(n + 1)\pi}. \tag{11}
\]

These are shown in Fig. 2, and are generally a good approximation to the exact solution of the system (4).

It is clear here that trajectories with odd and even \( n \), which approach the origin from different sides, will behave very differently, and in particular will have very different scaling for low \( \gamma \). In particular,

- for odd-\( n \) trajectories, in the tunnelling limit

\[
p_z^{sr} \approx \frac{F}{\omega} \frac{\gamma^2}{(n + 1)2\pi} = \frac{\gamma \kappa}{(n + 1)2\pi}, \tag{12}
\]

and the kinetic energy scales as \( \gamma^2 \) for a fixed target species, whereas

- for even-\( n \) trajectories

\[
p_z^{sr} \approx \frac{F}{\omega} \frac{2}{(n + 1)\pi}, \tag{13}
\]

and the kinetic energy is a constant fraction of \( U_p \), as found previously [25, 26]. This scales as \( \gamma^{-2} \).
These differences are grounded in much simpler scaling considerations. For even-\(n\) trajectories, the centroid of the oscillation must advance past the ion by twice the quiver radius \(z_{\text{quiv}} = F/\omega^2\) plus the tunnel length \(z_{\text{exit}} = 2\gamma^2 z_{\text{quiv}}\) within the given number of laser periods, which implies a scaling of the form
\[
p_{\text{z}} \sim \frac{2z_{\text{quiv}} + z_{\text{exit}}}{T} \approx \frac{2F/\omega^2}{2\pi/\omega} \sim \frac{F}{\omega},
\]
and an energy which scales as \(\gamma^{-2}\). (Further, this suggests that the small observed deviations from this exponent [1, 13] could also be explained by a shifted power law to account for the tunnel exit, as confirmed in Ref. 40.) For the odd-\(n\) trajectories, on the other hand, the centroid must only advance by the tunnel length in a multiple of a laser periods, and the scaling reflects this:
\[
p_{\text{z}} \sim \frac{z_{\text{exit}}}{T} = \frac{I_p/F}{2\pi/\omega} \sim \frac{I_p/\omega}{F}. \tag{15}
\]
Thus, the fixed distance to cover in an increasing amount of time gives these trajectories their very low momenta at long wavelengths. Indeed, for argon in a 3.1 \(\mu\)m field of intensity \(10^{14}\) W/cm\(^2\), as in Ref. 32, the highest odd-\(n\) momentum is \(p_\gamma \approx 0.02\) a.u. This corresponds to a minimum energy of 8 meV, which is consistent with the observed momentum spread of the ZES.

The difference in scaling behaviour also suggests avenues of experimental research for testing this connection, as well as for probing the internal structure of the ZES. In particular, it’s desirable to have experiments which increase the energy scale of the ZES and lift it above the consistent-level of the current experimental resolution, so that its details can be better examined. If it is caused by soft-recolliding trajectories of this nature, then its energy should scale as \(\gamma^2 I_p\), which points the way to experiment.

This scaling is fairly unfavourable, since it is also necessary to keep \(\gamma\) small to remain in the tunnelling limit. This means, then, that the ZES is best probed using high-\(I_p\) targets, of which the most natural is He\(^+\) ions – either as an ionic beam or prepared locally via sequential ionization or a separate pre-ionizing pulse. This brings a four-fold increase in \(I_p\) compared to hydrogen, and allows for a wider range of intensities and wavelengths which keep \(\gamma = \kappa \omega / F\) small but \(p_{\text{z}}^2 \sim \gamma I_p = \kappa^2 \omega / F\) large enough to be directly measured.

Finally, we note that the momentum ratios between the two families of trajectories form universal sequences independent of the system’s parameters: \(3/5, 5/7, 7/9, \ldots\) for even-\(n\) trajectories and \(1/2, 2/3, 3/4, \ldots\) for odd-\(n\) ones. The latter sequence should be difficult to resolve using current experimental setups but, if observed, would allow a richer window with which to observe the tunnel exit distance [40].

It is also important to point out that, irrespective of the precise mechanism which translates the soft-recolliding trajectories into peaks in the photoelectron spectrum, this mechanism should apply equally well to both series of trajectories. As pointed out above, quantum-orbit approaches increase their associated amplitude via imaginary parts of the action, whereas classical-trajectory approaches give photoelectron peaks through dynamical focusing near the soft recollisions. In either case, the dynamical similarity between the two series of recollisions, evident in Fig. 1, should cause similar results for both. The reason the odd-\(n\) trajectories have not appeared explicitly so far seems to be only their very low energy.\(^1\)

## II. ANALYTICAL R-MATRIX THEORY

We will now give a brief recount of ARM theory, as developed in Refs. 19, 20, emphasizing the features that provide initial conditions for the complex-valued quantum orbit trajectories, thereby leading to branch cuts in the complex time plane.

The \(R\)-matrix approach was adapted from nuclear physics [41] to model collisions of electrons with atoms [42] and molecules [43], and it is designed to deal with electron correlation effects by confining full many-body dynamics to the interior of a sphere around the system, where they are most important, and using a single-active-electron approximation outside it. In a strong-field context, this permits a fuller account of multi-electron effects [44, 45], and it also allows a smoother matching between the WKB asymptotics of the bound states near the ion with the perturbing effect of the ion’s potential on the continuum wavefunction on the outside region where this effect is small.

The effect of the ion can be accounted for rigorously, in the outer \(R\)-matrix region, by using the eikonal approximation [34, 35] on the usual Volkov states, where the phase and amplitude of the wavefunction are approximated by the first terms in a semiclassical series in powers of \(h\). This approximation yields continuum time-dependent wavefunctions of the form
\[
\langle \mathbf{r} | p_{\text{EVA}}(t) \rangle = \frac{1}{(2\pi)^{3/2}} e^{i\mathbf{p} \cdot \mathbf{A}(t)} \tau^{-\frac{1}{2}} \int_t^\tau e^{-i \int_{\tau'}^\tau U(\tau', \mathbf{r}, \mathbf{p}, t)} d\tau', \tag{16}
\]
where \(U\) is the ion’s electrostatic potential, and
\[
\mathbf{r}_I(\tau; \mathbf{r}, \mathbf{p}, t) = \mathbf{r} + \int_t^\tau (\mathbf{p} + \mathbf{A}(\tau')) d\tau' \tag{17}
\]
is the laser-driven trajectory that starts at position \(\mathbf{r}\) at time \(t\) and has canonical momentum \(\mathbf{p}\). These eikonal-Volkov states are (approximate) solutions of the time-dependent Schrödinger equation with the Hamiltonian
\[
H = \frac{1}{2} \mathbf{p}^2 + U(\mathbf{r}) + \mathbf{r} \cdot \mathbf{F}, \tag{18}
\]
or, in other words, they are propagated in time as
\[
| p_{EVA}(t) \rangle = U(t, t') | p_{EVA}(t') \rangle \quad \text{for } t > t' \tag{19}
\]
where the propagator \(U(t, t')\) obeys the (approximate) Schrödinger equation
\[
\frac{\partial}{\partial t} U(t, t') = H U(t, t'), \quad \text{with } U(t, t) = 1. \tag{20}
\]

\(^1\) In addition, if the position of the tunnel exit is dropped from the analysis then all odd-\(n\) trajectories will degenerate to zero energy, which helps confound the situation.
The quantity of interest is the photoelectron momentum wavefunction is correspondingly split into an inner and outer wavefunctions. This carries the problem that the hamiltonian is no longer hermitian in either region (as the usual integration-by-parts proof leaves uncanneld boundary terms), so the resulting system has two non-hermitian Schrödinger equations coupled through their boundary conditions.

The problem is rigorously addressed by introducing a ‘hermitian completion’ of the hamiltonian, by means of the Bloch operator

\[ L = \delta(r-a) \left( \frac{\partial}{\partial r} + \frac{1-b}{r} \right), \]  

for which \( H+L \) is hermitian in the inner region and \( H-L \) is hermitian in the outer region, with the Bloch operator cancelling out the boundary terms in the usual integration by parts. The system can then be re-expressed as two coupled, hermitian, inhomogeneous Schrödinger equations:

\[
\begin{align*}
\frac{i}{\hbar} \frac{\partial}{\partial t} \Psi_{\text{in}}(r, t) &= (H+L)\Psi_{\text{in}}(r, t) - L\Psi_{\text{out}}(r, t) \quad (22a) \\
\frac{i}{\hbar} \frac{\partial}{\partial t} \Psi_{\text{out}}(r, t) &= (H-L)\Psi_{\text{out}}(r, t) + L\Psi_{\text{in}}(r, t). \quad (22b)
\end{align*}
\]

In particular, since the Bloch term \( L\Psi \) is local to the boundary, we can implement the boundary conditions by substituting the wavefunction from the other side of the boundary in both equations, which then acts as a source term. The solutions to the coupled equations then automatically obey the boundary conditions.

Once with a well-formulated system, one can apply the relevant approximations. In practice, the equation for the inner region is not affected as long as the ionization rate is not too great, since then the Bloch term \( L\Psi_{\text{out}} \) can be neglected, or its main effects can be modelled by incorporating a ground-state depletion factor: furthermore, by an appropriate choice of the constant \( b \) in the Bloch operator, the ground state \( \Psi_g \) can be made an eigenstate of \( L \). (In particular, choosing \( b = 1/\kappa \) implies that \( L\Psi_g = -\kappa \delta(r-a)\Psi_g \).) Similarly, the Bloch term in the outer region’s hamiltonian can be neglected as the ionized wavefunction will generally be far from the boundary.

Given these approximations, one can then write down the formal solution to the outer Schrödinger equation (22b) as

\[ \Psi(t) = -i \int_{-\infty}^{t} U(t, t') L | \Psi_{\text{in}}(t') \rangle \, dt'. \]  

(23)

The quantity of interest is the photoelectron momentum amplitude at a time \( T \) long after the pulse is finished, which is then

\[
\begin{align*}
a(p) &= \langle p | \Psi(T) \rangle = -i \int_{-\infty}^{T} \langle p | U(T, t) L | \Psi_{\text{in}}(t) \rangle \, dt \\
&= -i \int_{-\infty}^{T} \langle p | \text{eSFA}(t) | L | \Psi_{g}(t) \rangle \, dt.
\end{align*}
\]

(24)

To calculate the spatial matrix element, we work in the position basis, so

\[
a(p) = -i \int \, dr \int_{-\infty}^{T} \langle p | \text{eSFA}(t) | r \rangle \langle r | L | \Psi_{g}(t) \rangle \\
= -i \int \, dr \int_{-\infty}^{T} \langle p | \text{eSFA}(t) \rangle \langle p + A(t) | r \rangle \langle r | L | \Psi_{g}(t) \rangle \\
\times e^{i \int_{\tau_{\text{in}}}^{t} f_{\text{p}}(p+\mathbf{A}(\tau))^2 d\tau} \times e^{i \int_{\tau_{\text{in}}}^{t} f_{\text{p}}(r) d\tau} \, d\tau \\
= -i \int_{-\infty}^{T} \langle p | \text{eSFA}(t) \rangle \langle p + A(t) | r \rangle \langle r | L | \Psi_{g}(t) \rangle \\
\times e^{i \int_{\tau_{\text{in}}}^{t} f_{\text{p}}(p+\mathbf{A}(\tau))^2 d\tau} \times e^{i \int_{\tau_{\text{in}}}^{t} f_{\text{p}}(r) d\tau} \langle \text{eSFA}(t) | r \rangle \langle r | L | \Psi_{g}(t) \rangle.
\]

(25)

This calculation produces, then, an ionization amplitude \( a(p) \) in the form of a temporal integration of a phase factor

\[ e^{i S_{\text{V}}(t)} = \exp \left[ i \left( I_p t + \frac{1}{2} \int_{-T}^{T} (p + A(\tau))^2 d\tau \right) \right], \]  

(26)

coupled the spatial and temporal integrations in a complicated fashion. This factor, moreover, is crucial in ensuring that the resulting amplitude is independent of the (unphysical) boundary radius \( a \).

To disentangle both integration steps, one first performs the temporal saddle-point integration, with an \( r \)-dependent result since the phase now includes a spatial term \( e^{i A(r)} r \). The resultant saddle point \( t_s \) is generally not far from the standard SFA saddle \( t_s = t_0 + i\tau \), which obeys

\[ \frac{1}{2} (p + A(t_s))^2 + I_p = 0. \]  

(28)

Moreover, the variations in \( t = t_s \) in the Coulomb correction term (27) exactly cancel out the variation with respect to \( a \) in the ground-state wavefunction [see 19, 20, 24].

The result of this matching procedure [19, 20, 24] is a simple expression for the ionization amplitude with most factors evaluated at the complex saddle-point time \( t_s \) of (28),

\[
a(p) = e^{i \tau_{\text{in}} t_s} e^{-\frac{1}{2} \int_{-T}^{T} (p+\mathbf{A}(\tau))^2 d\tau} \\
\times e^{-i \int_{-T}^{T} f_{\text{p}}(p+\mathbf{A}(\tau)) d\tau} F(p),
\]

(29)

where \( t_s = t_0 - i/\kappa^2 \) and the final amplitude will be a sum over all saddle points \( t_s \) with positive imaginary part.
In this expression the spatial factors have been incorporated into a shape factor
\[
R(p) = \frac{i\kappa^2}{\sqrt{2\pi V(t_0)}} \int d\Omega e^{-i \int_{t_0}^{t} U(\tau) p + A(\tau) d\tau} d\tau 
\times e^{-i(p+A(t_s))\cdot r} |\langle \psi_0 | r \rangle|_{r=a},
\]
which is independent of a [19, 20, 24]. This shape factor is essentially the Fourier transform of the ground state over the spherical boundary; in this sense it is analogous to the planar boundary used in partial Fourier transform over the spherical boundary; in this sense it is analogous to the planar boundary used in partial Fourier transform approaches [47].

The ARM ionization amplitude Eq. (29) is similar to the SFA result, and it admits a clear quantum-orbit trajectory [36]. The electron is ionized at time \( t_s \) and propagates to its detection, at real and large time \( T \), with velocity \( p + A(t) \) and position
\[
r_{cl}(t) = \int_{t_0}^{t} (p + A(\tau)) d\tau.
\]
Along the way, it acquires ‘phases’ given by the exponentiated action of the different relevant energies: \( e^{i\int_{t_0}^{t} \tau_s \cdot t} \) from the bound energy before ionization, \( e^{-i \int_{t_0}^{t} (p+A(\tau))^2 d\tau} \) from the kinetic energy after ionization, and \( e^{-i \int_{t_0}^{t} U(r_{cl}(\tau)) d\tau} \) from the Coulomb interaction. It is important to remark that these factors are no longer pure phases since the exponents are now complex, which greatly affects their amplitude and indeed completely encodes the (un)likelihood of the tunnelling process.

The complex integrals in Eq. (29) are complex contour integrals which can be taken, in principle, over any contour which joins both endpoints. In practice, the standard contour goes directly down from \( t_0 \) to its real part \( t_0 \) and then along the real axis until the detection time \( T \), as shown in Fig. 3. This conveniently separates the imaginary part of the contour, which yields an amplitude reduction \( e^{i\int_{t_0}^{t} \tau_s \cdot t} e^{-i \int_{t_0}^{t} (p+A(\tau))^2 d\tau} \) that encodes the tunnelling probability, and the normal propagation along the real time axis. As we shall see later, when the Coulomb interaction is included over one or more laser periods, this choice of the second leg of the contour is no longer necessarily ideal or even allowed.

The main effect of the matching procedure is that the \( r \)-dependent laser-driven trajectory (17) has been replaced by a classical trajectory of Eq. (31) starts at the origin, but this trajectory is only integrated over, in the Coulomb correction factor
\[
\exp \left(-i \int_{t_0}^{t} U(r_{cl}(\tau)) d\tau \right),
\]
from a time \( t_s = t_0 - i/\kappa^2 \) just under the saddle point. This shift arises here rigorously as a result of matching the outer-region wavefunction to the WKB asymptote of the bound wavefunction. Since its origin is intrinsically spatial, it is preferable to other regularization procedures such as the ionization-rate-based scheme of Ref. 13.

Finally, it is important to note that the process that leads to the Coulomb correction factor (32) is little more than the analytic continuation of the original factor (27), which appeared in the initial real-valued temporal integral (25). This uniquely determines the trajectory to use for the Coulomb correction, with the initial conditions set by the matching procedure. The trajectory \( r_{cl}(t) \), along which the Coulomb correction is integrated, obeys the laser-only equation of motion,
\[
\dot{r}_{cl}(t) = -F(t),
\]
as opposed to the full equation (including both the laser and the Coulomb field) used in the CCSFA approach [15–18]. This is a direct consequence of the appearance of \( r_{cl} \) in the EVA wavefunction (16). Work to include the effect of the ion on the trajectory should ideally be directed at its inclusion at the level of this wavefunction.

The initial conditions are also different to those used in the CCSFA approach. In ARM theory, the initial position is obtained from first principles and it is real at the entrance of the tunnelling barrier instead of its exit, as is imposed externally on the CCSFA trajectory. The consequences of this can be dramatic, as we show below, and among other things they preclude certain choices of integration contour in (32). In this light, calculating semiclassical trajectories for the full equation of motion with the correct initial conditions in complex time and space appears to be a far more difficult task.

In the next section we describe the origin of these difficulties, the mathematical challenges that arise, and how they can be addressed within the ARM theory.

FIG. 3. The time contour for integrating the exponents in Eq. (29) is usually taken from \( t_s \) down to its real part \( t_0 \) and then along the real axis until the detection time \( T \).

III. EMERGENCE OF TEMPORAL BRANCH CUTS

The analytical \( R \)-matrix theory allows us, then, a trajectory-based approach for accounting for the effect of the ionic potential on the photoelectron. Here the potential is integrated over the electron’s complex-valued trajectory (31) to give the correction factor (27), which now has a non-trivial amplitude. The trajectory starts at a real position, \( r_{cl}(t_s) \approx -2/\kappa \), but from then onwards both the integrand and the integration time are complex, so the position is therefore complex.

The imaginary part of the position has two main sources. The first is along the transverse direction, since any amount of real-valued transverse momentum \( p_\perp \) will accumulate an imaginary transverse position \( \int p_\perp \tau \) between the complex-valued \( t_s = t_0 + i\tau \) and any real time \( t \), from the ‘tunnel exit’ \( t = t_0 \) onwards. The longitudinal position, on the
other hand, also obtains imaginary components through the integral of the vector potential, which is now explicitly complex valued, so the end result is the nonlinear dependence shown in Fig. 4.

Since the integrand in (31) is real for real times, this imaginary position will not change along the real time axis, so it will remain present until the electron is detected at a large time $T$, at which the real position will be much larger. During a recollision, however, the real position becomes small. At this time, the imaginary coordinate dominates the position, which becomes an issue when calculating the ion’s electrostatic potential. The simplest choice for that is the Coulomb potential,

$$U(r) = \frac{1}{\sqrt{r^2}} = \frac{1}{\sqrt{x^2 + y^2 + z^2}},$$

which is analytical in this form. Other potentials are also tractable, as long as they are analytical functions on the real axis, but pose similar mathematical challenges. For the Coulomb potential, the extension procedure requires the use of a square root, which in general poses at most an integrable singularity, but for complex arguments it has a branch cut along the ray $r^2 \in (-\infty, 0)$ which cannot be ignored.

This branch cut is reached, precisely, on recollisions where the imaginary part dominates a nonzero real part. Indeed, the squared position can be decomposed as

$$r^2 = \text{Re}(r)^2 - \text{Im}(r)^2 + 2i \text{Re}(r) \cdot \text{Im}(r),$$

which means that, when $\text{Im}(r)^2 > \text{Re}(r)^2$, the trajectory will reach the branch cut at the point where the projection $\text{Re}(r) \cdot \text{Im}(r)$ changes sign. This is marked by a discontinuous change in the square root $\sqrt{r^2}$, with a sudden change in the sign of the imaginary part $\text{Im}(\sqrt{r^2})$. If one integrates across this discontinuity, the dependence on $t$ of the Coulomb integral (27) ceases to be analytic, and one loses the freedom that allowed the real contour of (25) to be deformed to pass through the saddle point $t_s$ in the first place, and the results are no longer meaningful.

The solution to this problem is to view the entire potential as a function of time,

$$U(t) = \frac{1}{\sqrt{r_{cl}(t)^2}},$$

as a single analytical function of the complex-valued variable $t$. The branch cuts in $U$ are imprinted on the time plane via the conformal mapping $t \rightarrow r_{cl}(t)^2$. We show in Fig. 5(a) an example of the Coulomb potential’s behaviour, as a contour map of the function $\sqrt{r_{cl}(t)^2}$ (which has the branch cut structure of $U$ but omits its singularities). The essential features of this function are the branch cuts, which are sketched in Fig. 5(b) in red. In particular, the standard integration contour of Fig. 3 – straight down from $t_s$ and then along the real axis, shown dotted in Fig. 5(b) – can indeed cross the branch cuts when the electron returns near the ion.

This means that to preserve the analyticity of (27) one must deform the integration contour away from the real time axis until the integrand is continuous and analytic. This will correspondingly change the way the complex position $r_{cl}(t)$ moves in space, with the main effect of minimizing the imaginary part of the position at the time of recollision; this is exemplified in Fig. 6.

The relationship between the chosen temporal contour and the corresponding trajectory in complex position space, particularly along $z$, is in general complicated and hard to visualize. Similarly, the final momentum $p$ has a strong effect on the potential $U(r_{cl}(t))$ as a function of time, sometimes very sensitively (such as near a soft recollision). These variables are all intertwined, with the momentum determining the branch cut structure and therefore the possible contours on both the time and space complex planes.

To help disentangle these relationships, we have developed a software package [37] which enables real-time visualization of the effect of a particular choice of contour and pose conflicting demands, and numerical evaluation via integration of a Coulomb kernel fails to give analytical results. We will analyse these differences in detail in a future publication.
momentum on the space trajectory and on the temporal branch cut structure. This software is described in detail in Ref. 38 and we encourage the reader to use its visualization tools to explore the implications of our results.

IV. TIMES OF CLOSEST APPROACH

We see, then, that the existence of branch cuts which can cross the real axis can preclude the use of the standard integration contour for the integral in (27), and one needs to choose a contour which passes through the ‘slalom gate’ left by the branch cuts of $U(t)$ as in Fig. 5(a). If only a few momenta are involved then this can be done on a case-by-case basis, but the computation of photoelectron spectra requires a more programmatic approach, which is able to automatically choose the correct contour for each given momentum.

To obtain this approach, we examine in detail the space between the two branch cuts, as shown in Fig. 7. Each branch cut is a contour of constant $\text{Re}(\sqrt{r_c(t)}) = 0$, which means that the neighbouring contours must closely follow its direction, and circle around it when it terminates at the branch point. In the ‘slalom gate’ configuration of Fig. 5(a), the only way to combine the curvatures of the contours near the facing branch cuts is to have a saddle point in between them. This saddle point is the crucial object which enables the automatic choice of a contour which avoids the branch cuts, as it is ideally situated between them. Moreover, it has a deep physical and geometrical significance, which we explore in this section.

It is clear in Fig. 7 that any contour which crosses the complex $t$ plane from left to right must have a real distance to the origin $\text{Re}(\sqrt{r_c(t)})$ which decreases, reaches a minimum, and then increases again. For contours which cross the branch cut, this minimum is zero, and it is accompanied by a discontinuous change in the imaginary part. For a path crossing through the saddle point, on the other hand, the minimum of $\text{Re}(\sqrt{r_c(t)})$ is at its maximum value, and this minimum occurs precisely at the saddle point.

For this reason, we call the saddle point the time of closest approach, and we label it $t_{CA}$. To be precise, then, a contour that passes through $t = t_{CA}$ maximizes the minimum value of the real part of the distance to the origin, $\text{Re}(\sqrt{r_c(t)})$. Intuitively, it permits the furthest possible approach to the ion.

Similarly, when calculating the Coulomb potential along such a contour, this choice minimizes the maximum value
of the real part of $1/\sqrt{r_{cl}(t)^2}$ and its absolute value (for valid contours which do not cross the branch cuts), so that the Coulomb interaction is kept as bounded as possible. As long as the potential $U(r_{cl}(t))$ stays continuous and analytic, this is not essential, as the integral in (27) does not change. However, this contour optimizes the applicability of the approximations that led to (27), and it admits the clearest physical interpretation by keeping the imaginary part of the position within the tightest bound possible at the points where this is necessary. Additionally, it minimizes the difficulties faced by numerical integration routines.

To find the saddle points, one simply looks for zeros of the derivative of $\sqrt{r_{cl}(t)^2}$. This can be further reduced to the zeros of $\frac{d}{dt} [r_{cl}(t)^2]$, so the criterion is simply

$$r_{cl}(t_{CA}) \cdot \mathbf{v}(t_{CA}) = 0.$$ (37)

This equation is deceptively simple, and one must remember that the left-hand side is a complex-valued function of time through Eq. (31). Nevertheless, it has a compelling physical interpretation, for if a classical electron passes near the nucleus then it is closest to the origin when its velocity and its position vector are orthogonal.

In this spirit, then, it is worthwhile to investigate the classical solutions of (37) before exploring the solutions in the complex quantum domain. As we shall see, both domains exhibit rich geometrical structures which are closely related to each other and, moreover, the times and moments of soft recollisions emerge naturally as crucial geometrical points within both structures. After exploring the geometrical implications in both contexts, we shall use this knowledge to automatically generate correct integration contours for any momentum.

### A. Classical times of closest approach

The classical closest-approach times $t_{CA}^{\text{class}}$ are naturally defined via

$$\text{Re} [r_{cl}(t_{CA}^{\text{class}}) \cdot \mathbf{v}(t_{CA}^{\text{class}})] = \text{Re} [r_{cl}(t_{CA}) \cdot \mathbf{v}(t_{CA})] = 0.$$ (38)

The problem in using them as a tool, however, is that both of their defining equations, (37) and (38), have several other solutions, and these are not always distinguishable from the desired closest-approach times. In particular, the turning points of the classical trajectory, away from the core, are also solutions of (37), since they are also extrema of $r^2$. Thus, for instance, the surface in Fig. 5(a) contains saddle points at $\omega t \approx \pi/4$ and $\omega t \approx 3\pi/4$, which correspond to the turning points shown in Fig. 6 to the right and left of the position at $t_0$, respectively. Thus, to be able to use the closest-approach times as an effective tool to avoid the branch cuts one needs to distinguish the crucial mid-gate $t_{CA}$ points from the other solutions.

In certain cases this is easy, such as for on-axis collisions with $p_\perp = 0$. Here (38) reads

$$\text{Re} [z_{cl}(t_{CA}^{\text{class}}) v_{z}(t_{CA}^{\text{class}})] = 0,$$ (39)

and it solutions cleanly separate into turning points, with $v_z(t_{CA}^{\text{class}}) = 0$, and collisions with $z_{cl}(t) = 0$, as shown in Fig. 8(a). The turning points can additionally be classified as minima and maxima of $r_{cl}(t)^2$, shown respectively in green and red, by evaluating the sign of $\frac{d^2}{dt^2} r_{cl}(t)^2$. At nonzero $p_\perp$, it is the collisions that will turn into useful closest-approach times.

Within this context, the classical soft recollisions studied in Section 1 appear naturally as the intersection between these two curves: the times when both $v_z(t) = 0$ and $z_{cl}(t) = 0$. Moreover, at these intersections the number of available roots changes. Thus, as $p_\perp$ is swept up across the intersection marked a in Fig. 8(a), an inward
turning point turns into an outward turning point flanked by two closest-approach points. The classical trajectory exhibits exactly this behaviour, as shown in Fig. 9(a), with this change in \( p_z \).

The roots of (39) can also merge at the extremes of the sinusoidal turning-point curve of Fig. 8(a). At these points, the longitudinal momentum becomes greater than the oscillation amplitude \( F/\omega \), and the velocity \( v_z(t) = p_z - \frac{F}{\omega} \sin(\omega t) \) no longer changes sign. The resulting behaviour of the trajectories is shown in Figs. 9(b) and (c), and resembles pulling a winding string until the turns are straight.

The closest-approach solutions of (38) become more interesting when one allows a nonzero transverse momentum \( p_x \). Here the solutions form a single coherent surface, shown in Fig. 8(b), that consists of a number of bounded lobes joined together at the soft recollisions, which locally look like cones. Thus, it is possible to continuously connect any two roots of (38) via a path on the surface. More specifically, the inward turning points and the recollisions shown in green in Fig. 8(a) can be smoothly connected via the \( p_z \neq 0 \) component of the surface, which precludes the existence of a simple criterion to distinguish one from the other in the general case.

On the other hand, the outward turning points can still be distinguished, as they are local maxima of \( r_{cl}(t)^2 \). These maxima are shown in red in Figs. 8(a) and (b), and they form the “left-facing” side of the surface in Fig. 8(b). More specifically, any horizontal line of constant momentum must enter the surface through a maximum (red) and leave it through a minimum (green), because the minima and maxima must alternate for any given trajectory. Thus, the red (maximum) side of the surface points towards negative \( t \), and the green (minimum) side points towards positive \( t \).

At the boundary between both parts of the surface, a maximum and a minimum merge and disappear, and the trajectory will then behave as shown in Fig. 9(b), (c) or (d), depending on which direction the boundary is approached (i.e. towards positive \( p_x \), negative \( p_x \), and increasing \( p_x \), respectively). Horizontal lines of constant momentum will be tangent to the surface at this boundary, and the corresponding trajectory will have a double root of (38).

**B. The quantum solutions**

The quantum solutions have a richer geometry, with an additional dimension, imaginary time, to be occupied. The main effect of this is to increase the number of available solutions; while in the classical case two real solutions of (38) can merge and disappear, in the quantum case the
complex solutions of (37) are not lost, but will move into imaginary time and remain present.

In general, the quantum solutions will be close to the classical ones when the latter exist. As one approaches the end of a lobe on the classical solution surface of Fig. 8(b), however, the quantum solutions approach each other close to the real axis and then diverge into positive and negative imaginary time, keeping a relatively constant real part. If one then projects this to real times, the result is a pair of surfaces which closely follow the red and green parts of the classical surface, and then diverge into roughly parallel planes as they reach the boundary. We show this behaviour in Fig. 10.

The first few closest-approach solutions are relatively easy to handle, and depend smoothly on the momentum. This includes the first minimum and maximum of $r_{cl}(t)^2$, like the ones in Fig. 5(a), the birth time $t_s$ itself, and a conjugate solution with negative imaginary part which should be ignored. These solutions occupy specific regions of the complex $t$ plane, as shown in Fig. 11(a), and can be consistently identified. Moreover, these solutions exhibit close approaches at $\omega t \approx \pi/2$ and $\omega t \approx 3\pi/2$ which are the quantum counterparts of the classical maximum-minimum mergers shown in Figs. 9(b) and (c). These are evident in Fig. 10 as the converging surfaces at those times, and are of relatively limited interest.

The most important $t_{CA}$ close approaches occur at and near the soft recollisions, shown inside the gray rectangle of Fig. 11(a) and in Fig. 11(c), with a complicated momentum dependence which we explore below. In the quantum domain, soft recollisions again represent interactions between three different closest-approach roots. Unlike the classical domain, however, the roots do not merge; instead, two of them move into imaginary time after a three-way avoided collision, shown in Fig. 11(c) between the points marked 9 and 10. The proximity between the multiple saddle points marks the increased time the electron spends near the ion in the neighbourhood of a soft recollision.

More interestingly, this three-way collision marks a crucial topological change in the configuration of the branch cuts associated with the recollision, as shown in Fig. 12. Each of the outer saddle points, $t_{CA}^{(1)}$ and $t_{CA}^{(3)}$, has a pair of branch cuts associated with it, in the same ‘slalom gate’ configuration as in Fig. 7, and these go off into imaginary time. However, the way in which they do so changes as the longitudinal momentum $p_z$ passes the momentum $p_z^2$ of the soft recollision.

For $p_z$ below $p_z^2$, as in Fig. 12(a), the branch cuts loop back to imaginary time without crossing the real time axis. As with the low-momentum trajectory of Fig. 9(a), the trajectory does not quite reach the collision, and the associated branch cuts do not force a change of contour. At $p_z = p_z^2$, however, the branch cuts touch and reconnect, and for $p_z > p_z^2$ the topology changes to the one shown in Fig. 12(b). Here the trajectory does pass the core, and the associated branch cuts do cross the real axis, forcing the integration contour to change and pass through the gates.
This process has profound implications for the ionization amplitude, because these drastic changes in the integrand occur precisely when it is largest. Thus, choosing the wrong contour in this region accounts for the largest contributions to the integrand, with a correspondingly large effect on the integral. More surprisingly, once the contour is forced to pass through the ‘gate’ $t_{CA}$, for $p_z$ just above $p_z^{cr}$, their contributions have the effect of suppressing the ionization amplitude there.

To see how this comes about, consider the integral $\int U(r_c(t))dt$ for the configuration of Fig. 12(a). Here $\sqrt{r_c(t)}$ has a minimum at the central saddle point, $t_{CA}^{(2)}$, and this translates into a maximum of $1/\sqrt{r_c(t)}$ which dominates the integral. At this point, the approach distance $r_s = \sqrt{r_c(t_{CA}^{(2)})}$ is dominated by a modest and positive imaginary part. This means that $U_s = -1/r_s$ is large and imaginary, and therefore the correction factor $e^{-i \int U dt}$ has a large amplitude.

On the other hand, in the configuration of Fig. 12(b) the integral is dominated by the ‘gate’ closest-approach times, for which $r_s' = \sqrt{r_c(t_{CA}^{(1)})} \approx \sqrt{r_c(t_{CA}^{(1)})}$ is mostly real and much smaller than $r_s$. The corresponding potential $U_s' = -1/r_s'$ is then large, real and negative, and $-iU_s'$ is along $+i$. However, here the line element $dt$ must slope upwards with a positive imaginary part to emphasize the contribution of the saddle point, and this then gives $-i \int U(r_c(t))dt$ a large and negative real part. This, in turn, suppresses the amplitude of the correction factor $e^{-i \int U dt}$.

This effect is visible in photoelectron spectra as a large peak just below the soft recollision, followed by a deep, narrow dip. In an experimental setting, the dip will almost certainly get washed out by nearby contributions unless specific steps are taken to prevent this, but the peak will remain. In addition, this effect mirrors the redistribution of population seen in classical-trajectory based approaches, where the peaks caused by dynamical focusing represent trajectories taken from other asymptotic momenta, whose amplitude is reduced.

We now turn to the momentum dependence of the closest-approach times near the soft recollision, which again presents interesting topological features. The main problem is illustrated in Figs. 11(b) and (c): the different solutions of (37) mix, and there is no longer any way to distinguish them from each other, as there was in the classical case. More specifically, traversing a closed loop in momentum space, like the semicircle shown in Fig. 11(b), will move the roots around in such a way that when one returns to the initial point the overall configuration is the same, but the saddle points have been permuted cyclically.

Topologically, this means that the surface defined by (37) (a two-dimensional surface in a four-dimensional space) does not separate into distinct components; instead, the surface has a single connected component after $\omega t = 3\pi/2$. On the other hand, the surface itself remains singly connected. Both of these behaviours are explored in Figs. S3 and S4 in the Supplementary Information [39].

This mixing behaviour is unusual in the quantum orbit formalism, where the norm is for rather elaborate indexing schemes to be possible [28, 48], partly because there is usually a single free parameter that governs the motion of the

FIG. 12. During a soft recollision, the quantum times of closest approach will perform a three-way close approach, like that shown in Fig. 11(c) at the first soft recollision between the points 9 and 10. At this close approach, the branch cuts associated with these saddle points will reconnect and change topologies, as shown in (a) and (b). This happens near, but not at, the classical soft-recollision momentum studied in Section I. At the point of the topological change, the outer saddlepoints $t_{CA}^{(1)}$ and $t_{CA}^{(3)}$ emerge from the classically forbidden region, and the real part of their kinetic energy $Re(\psi(t)^2)$ changes sign, as shown in (c) and (d). After the change, the outer saddlepoints do not require tunnelling to get to, and should be crossed by the integration contour. We show in (e) and (f) a sketch of the relevant branch cuts, analogous to Fig. 5(b), along with the appropriate integration contour for each topology. In (g) and (h) we show the corresponding trajectories in the complex $z$ plane for those contours. The motion along $z$ is similar to Fig. 9(a), with a modest imaginary part as in Fig. 4, and if the core is not reached does not represent a problem. For the slightly higher momentum of (h), however, the trajectory passes the origin and would cross the associated branch cut if taken along the dashed integration contour of (f), so the contour must be deformed to avoid it, as shown by the solid line. Here $p_z = 0.001$. 
saddle points. Here the control space is two-dimensional, which allows for nontrivial closed loops inside it, and this defeats the possibility of attaching any type of label to individual roots of $(\ref{eq:37})$.

Finally, an interesting consequence of the mixing between roots is that, at certain specific values of $p_\perp$ and $p_z$, the roots must merge, giving double roots of $(\ref{eq:37})$. However, this behaviour depends very sensitively on the momentum, and it can safely be ignored. In fact, the very difficulty of tagging the roots, caused by the mixing, makes finding the merge momentum an elusive numerical problem.

C. Navigating the branch cuts

Apart from its noticeable effects on the ionization amplitude, the topological change in the temporal branch cuts has an obvious effect on the integration contour required to produce a correct yield. The closest-approach times are a useful tool in identifying and crossing the branch-cut gates when they are present. However, some gates lead to dead-end regions which do not need to be crossed, which means that not all $t_{CA}$s are useful stepping points.

Thus, while the correct contour can always be chosen by hand given a specific branch cut configuration, it is also desirable to have an algorithm that will specify which ‘slalom gates’ the contour should cross, and in which order it should do so. Without such an algorithm, it is impossible to automate the choice of contour and the calculation of photoelectron spectra is impractical.

Such an algorithm is indeed available, and it is based on a geometrical fact shown in Figs. 12(c) and (d): the topological change in the branch cut connections that happens at a soft recollision comes together with a change in the sign of the real part of the squared velocity, $v(t)^2$, for the outer saddle points.

Thus, in the closed topology of Fig. 12(b), where the contour should pass through $t_{CA}^{(1)}$ and $t_{CA}^{(3)}$, the real kinetic energy $\text{Re}(v(t)^2)$ is positive at those saddle points. In contrast, for the open topology of Fig. 12(a), $\text{Re}(v(t_{CA}^{(1)})^2)$ and $\text{Re}(v(t_{CA}^{(3)})^2)$ are both negative, and the contour should ignore both of those saddle points.

The physical content of this criterion is quite clear: in the quantum orbit formalism, the classically forbidden regions are readily identified in the complex time plane as those regions where the kinetic energy $\frac{1}{2}v^2(t)$ is negative, or at least has negative real part. The undesirable saddle points of Fig. 12(a) therefore require the trajectory to tunnel towards the core to be reached. On the other hand, a formal proof of the simultaneity of the topological change with the emergence of the $t_{CA}$ from the ‘barrier’ is still lacking.

We display in Fig. 13 some sample integration contours produced with this criterion. In general, the navigation is straightforward, and there are never any problems when $p_\perp < 0$ or $p_z$ is sizeable, in which case contour looks as in Fig. 13(a). For near-recolliding electrons, on the other hand, the branch cuts do require more careful navigation, as we have seen.

In general, it suffices to take, in order of increasing $\text{Re}(t_{CA})$, those closest-approach times which (i) occur after ionization, (ii) have reasonably bounded imaginary part, and (iii) have positive kinetic energy. To this we add two exceptions: the first inward turning point, in $-\pi/2 < \omega t < \pi/2$, which helps avoid crossing regions where $\text{Re}(v(t)^2) < 0$ where this is not necessary; and the first closest-approach time, in $\pi/2 < \omega t < 3\pi/2$, when it can be consistently identified, which can sometimes have $\text{Re}(v(t_{CA})^2) < 0$ at extremely large momenta, but is nevertheless the correct choice in those cases.

Thus, a concrete set of rules for choosing a contour is taking those $t_{CA}$s for which

\[ \text{Re}(\omega t_{CA}) > \omega t_0 + \pi/5 \quad \text{and} \]
\[ -\frac{\pi}{2} < \text{Im}(t_{CA}) \leq \text{Im}(t_x) \quad \text{and} \]
\[ \text{Re}(v(t_{CA})^2) > -u, \]
\[ \text{or} \quad -\pi/2 < \text{Re}(\omega t_{CA}) < \pi/2 \quad \text{and} \]
\[ 0 \leq \text{Im}(t_{CA}) < \tau_T, \]
\[ \text{or} \quad \pi/2 < \text{Re}(\omega t_{CA}) < 3\pi/2 \quad \text{and} \]
\[ \text{Im}(t_{CA}) > 0, \]

where $u$ is an adjustable numerical precision, for additional flexibility, set by default to $10^{-8}$ a.u. These rules are relatively heuristic and they have a certain amount of leeeway around them, but they work well over the relevant region of photoelectron momentum to produce correct integration path choices.

FIG. 13. Sample integration contours produced by the $t_{CA}$ choosing algorithm described in the text. Most momenta are straightforward (a), but near-recollision momenta, like the one shown in Fig. 5, do require careful handling, as shown in (b). The algorithm correctly handles soft recollisions, (c), as well as higher momenta with harder recollisions (d).
Finally, we note that in certain very specific cases, close
to a soft recollision, the integration path is topologically
 correct but may pass near a singularity of the Coulomb
 kernel; future work aims at avoiding this problem.

V. RESULTS

We are now in a position to produce photoelectron spec-
tra. The yield is given by the amplitude in (29), taking
the integration of (32) to be over the \( t_{\ell a} \) chosen using the
hopping algorithm described above. The correctness of the
integration contour is reflected by the lack of discontinuous
changes in the final integrand, which are easily detected by
numerical integration routines when they are present.

In general, the inclusion of the Coulomb correction factor
(32) has the main effect of increasing the electron yield by
two or three orders of magnitude compared to the bare SFA
yield, which is a well known consequence of the Coulomb
interaction \([15,17,19]\), and is primarily due to the interac-
tions inside the classically-forbidden region.

This enhancement is particularly strong, and has a par-
ticularly strong variation, near the classical soft recollisions
\( p_z^{sr} \). As discussed above, these are accompanied by an ex-
treme enhancement for momenta on one side of \( p_z^{sr} \) and a
deep and narrow dip on the other. The presence of mul-
tiple saddle points in close proximity, which marks the in-
terpreted momenta in the calculations of states near the core, implies the
Coulomb correction must be large, but its precise con-
tribution depends sensitively on the details of the topological
transition at the soft recollision.

In the neighbourhood of such a soft recollision, the domi-
nating feature is a sharp ridge for very small transverse mo-
menta, as shown in Fig. 14, which terminates at \( p_z^{sr} \). This
ridge feature is similar to the cusps detected at low trans-
verse momenta in careful measurements of photoionization
spectra at long wavelengths \([32]\), which rise suddenly from
a gaussian background as \( p_z \) varies, though the measured
spectra have sharper cusps.

On the other side of the soft recollisions, i.e. for \( p_z > p_z^{sr} \),
this behaviour reverses, and the enhancement turns into a
strong suppression of ionization. This suppression is ev-
dent in Fig. 14, which contains two transitions closely
spaced at \( p_z^{sr} = 0.063 \text{ a.u.} \) and \( p_z^{sr} = 0.031 \text{ a.u.}; \) the in-
teractions between them create complex structures in their
immediate vicinity. These fine structures will most likely
be washed out in any experimental situation, but the spike
would be expected to remain.

The rapid change from enhancement to suppression of
the ionization signal at the topological transitions of Fig. 12
can be used to show their direct link with the classical
soft recollisions of Section I, by comparing their respective
wavelength scaling. To this end we plot in Fig. 15 the
variation of the on-axis ionization yield – at a small but
reasonable transverse momentum – with the laser wave-
length. The resulting ridges in the ionization yield closely
follow the scaling of the classical soft-recollision momenta
of Fig. 2, shown as red dots, which shows a strong link
between both structures. Similarly, the opposite scaling of
the two types of low-energy structure is amenable to ex-
perimental testing.

VI. CONCLUSIONS

We have seen how the analytical \( R \)-matrix theory gives
rise, from first principles, to a quantum-orbit picture of
strong field ionization which contains the Coulomb inter-
action with the ion as an added action in the phase. In this
picture the electron trajectory starts at the ion with a real
position, and as it travels through the classically forbidden

\[ \frac{\left| a(p_x, 0, p_z) \right|^2}{\left( a(p_x, 0, -p_z) \right)^2} \]

\[ |\alpha(p)|^2 \]

\[ \text{in an arbitrary logarithmic scale, as a function of the wavelength}
\]

\[ \lambda = 3.1 \mu\text{m}, \text{ with } \gamma = 0.31 \]

\[ \text{The Coulomb-correction has been integrated over 2.75 laser}
\]

\[ \text{periods. Recent experimental results at this wavelength \([32]\) show a}
\]

\[ \text{similar (if more pronounced) peak structure localized at small}
\]

\[ \text{longitudinal momentum.} \]

\[ \text{FIG. 14. Incoherent addition of the sub-cycle ionization yields,}
\]

\[ \frac{\left( \alpha(p_x, 0, p_z) \right)^2}{\left( \alpha(p_x, 0, -p_z) \right)^2}, \text{ ignoring the shape factor}
\]

\[ R(p) \]

\[ \text{for long wavelength fields (} \lambda = 3.1 \mu\text{m, with } \gamma = 0.31 \).
\]

\[ \text{The Coulomb-correction has been integrated over 2.75 laser}
\]

\[ \text{periods. Recent experimental results at this wavelength \([32]\) show a}
\]

\[ \text{similar (if more pronounced) peak structure localized at small}
\]

\[ \text{longitudinal momentum.} \]

\[ \text{FIG. 15. Variation of the on-axis ionization amplitude } |\alpha(p)|^2,
\]

\[ \text{in an arbitrary logarithmic scale, as a function of the wavelength}
\]

\[ \lambda = 3.1 \mu\text{m, with } \gamma = 0.31 \]

\[ \text{The sudden drops}
\]

\[ \text{in amplitude of Fig. 14 shift along the momentum axis with a}
\]

\[ \text{scaling that closely matches the classical soft-recollision trajec-
\]

\[ \text{tories, shown as red dots. Here the transverse momentum }
\]

\[ p_z \]

\[ \text{has been chosen so that the transverse coordinate of the classi-
\]

\[ \text{cal trajectory has a small but positive value, } x = 1.07 \frac{\mu\text{m}}{\pi}, \text{ at the}
\]

\[ \text{first soft recollision at } \omega t \approx 2\pi, \text{ to avoid the hard singularity of the}
\]

\[ \text{Coulomb kernel.} \]
region it acquires an imaginary component.

This imaginary component is not generally a problem, but it can dominate the trajectory near recollisions, in which case the Coulomb interaction can develop a discontinuous change in sign. This marks a branch cut which must be carefully handled, by treating the Coulomb interaction \( U(x(t)) \) as an analytic function on the complex plane, with branch cuts inherited from the spatial \( U(r) = -1/\sqrt{r^2} \), which the temporal integration contour must avoid.

The key tool for avoiding these branch cuts in the complex plane are the times of closest approach, which satisfy the complex equation \( r(t_{cl}) \cdot \sqrt{v(t_{cl})} = 0 \), and which are always present in the middle of each branch-cut gate. These times of closest approach have a rich geometry of their own, in the complex quantum domain as well as in the real-valued simple-man’s model. Moreover, the soft recollisions responsible for the Low Energy Structures are embedded in this geometry and arise naturally within both formalisms.

Using the times of closest approach, we have developed a consistent algorithm which enables the programmatic choice of a correct integration contour for all momenta, despite topological changes which can be quite brusque as the momentum crosses a soft recollision.

In particular, this formalism incorporates in a natural way the known series of trajectories which gives rise to the Low-Energy Structures, but it also predicts a second series of trajectories at much lower momentum. These trajectories do not appear in theories which neglect the tunnel entrance, which explains why they have so far been overlooked, but they should contribute to the recently discovered Zero-Energy Structures [31–33].

More broadly speaking, our work serves as a roadmap for the difficulties that must arise in a full first-principles semiclassical theory of ionization, and how they might be resolved. ARM theory, in its current form, uses only the laser-driven trajectory and does not incorporate the effect of the ion’s Coulomb potential on the trajectory itself. However, it is also clear that any first-principles attempt to include the Coulomb interaction at that level will be subject to the same imaginary-position properties as ARM theory, which makes the calculation of the full trajectory a nontrivial problem. In particular, such a theory will be subject to the same temporal branch cuts as ARM theory, without the benefit of the easily-found ARM closest-approach times to help navigate them.

In addition, by identifying mechanisms which should contribute to the observed Zero Energy Structures, we are able to propose experiments which can increase its energy scale and bring its details within reach of current experimental capabilities. In particular, the energy scaling of odd-order soft-recollision trajectories as \( \gamma \to 0 \) suggests that experiments with harder targets, such as \( \text{He}^+ \), should help elucidate the origin of these structures.

Furthermore, this trajectory-based explanation opens the door to testing via schemes which directly alter the shape of the trajectory. This includes variation of the pulse width, which is known to be a critical variable [26] along with the carrier-envelope phase, but it opens the door to testing using elliptical pulses or small amounts of second or third harmonics to shift the positions of the trajectories responsible for the structures.

This work thus provides a toolbox of approaches with which to understand the semiclassical dynamics of low-energy photoelectrons in the tunnelling regime, which should inform other low-energy ionization phenomena [49–51] as well as streaking-based experiments [52] in that regime.

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