The structure of ionizing electron trajectories for hydrogen in parallel fields

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Abstract

Classical trajectories of an electron escaping from a hydrogen atom in parallel electric and magnetic fields exhibit strikingly diverse and complex behavior. We study the qualitative structure of these trajectories. Specifically, we present a symbolic algorithm that allows one to compute the number of radial oscillations of the electron before it escapes, and to determine whether or not each such oscillation encircles the nucleus. The algorithm applies to a large and prominent (but not exhaustive) family of ionizing trajectories.

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1 Introduction

In previous work[1,2], we proposed an experiment in which hydrogen atoms, placed in external parallel electric and magnetic fields, are excited by a short laser pulse of high enough frequency that the energy of an excited electron exceeds the classical ionization barrier. The resulting flux of ionizing electrons is then measured by a detector placed downhill, i.e. in the direction of acceleration by the electric field. We predicted that one could observe a train of electron pulses striking this detector. The structure of this pulse train reflects fractal behavior within the chaotic dynamics of the ionizing electrons [3].

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Fig. 1. A prediction for the rate at which electrons, ionizing from hydrogen in parallel fields, strike a detector. The model assumes an initial classical ensemble of electrons moving away from the nucleus with constant energy and with exactly the same launch time. See Ref. [2] for greater detail. Several of the early time pulses are labeled, with their representative ionizing trajectories shown in Fig. 4.

The following qualitative description of the ionization process is helpful. First, the electron absorbs a photon from the laser pulse. The excited electron forms an outgoing wave, moving away from the nucleus in all directions. We model this wave by a classical ensemble of electron trajectories that begin at the nucleus and propagate outward in all directions. The frequency and duration of the laser pulse are such that all trajectories in this ensemble are launched at nearly the same time and have nearly the same energy. As time evolves, some of these trajectories find their way over a saddle in the potential energy surface that separates the Coulomb center from the ionization channel. These trajectories are subsequently accelerated toward the detector, striking it in a series of pulses (Fig. 1).

A natural question arises when looking at the picture of a pulse train (Fig. 1): What do the ionizing orbits associated with each pulse actually look like? The answer is shown in Fig. 4 for 29 early pulses. Our objective in this paper is to understand these pictures: (i) We seek a simple description of the qualitative shapes of the trajectories. (ii) We seek a set of rules that predicts these qualitative shapes and explains the relationships among them.

The first goal is easily accomplished. Along with the picture of each trajectory in Fig. 4, there is a string of dashes and ohs that record the trajectory's qualitative behavior. Each dash represents a portion of the trajectory that begins on the negative z axis (the dotted line) and returns to it without encircling the nucleus. Each oh represents a portion that does encircle the nucleus. The reader is invited to examine each $(-o)$-string (pronounced "dash-oh" string), reading it left to right, and sketch the corresponding orbit without looking at the picture. One will find that the $(-o)$-string, together with continuity of position and velocity, encapsulates the essential shape of the orbit.

The second goal can now be restated as: We seek a set of rules that permit us to predict the $(-o)$-strings directly, without recourse to pictures of the trajectories. In this paper, we develop a symbolic algorithm which accomplishes this goal for a large class of trajectories; for example, it applies to all but one of the trajectories shown in Fig. 4, i.e. it describes the trajectories associated with most of the early pulses in the chaotic pulse train. This algorithm is purely algebraic – it does not solve the differential equations. It is a lengthy algorithm, but it does its job, and we doubt there is a significantly simpler one.

The algorithm also explains patterns among the shapes of various trajectories.

These patterns are visible in Fig. 4 and are summarized by Facts 1 and 2 in Sect. 3.

The symbolic algorithm is stated without justification in Sect. 4. This section requires no background in symbolic dynamics. The justification is provided in Appendix A, which assumes some familiarity with maps, homoclinic tangles, and symbolic dynamics. The algorithm is based upon a new approach to homoclinic tangles, called homotopic lobe dynamics, which was introduced in earlier work [4]. Standard formulations of symbolic dynamics typically describe how an individual trajectory visits points in the phase plane. In contrast, homotopic lobe dynamics focuses on how a whole curve in the phase plane maps forward, thereby describing the evolution of a family of trajectories [5]. The algorithm we present takes the *phase space* description afforded by homotopic lobe dynamics and translates it into a *configuration space* description of orbits in terms of the $(-o)$-strings.

The paper has the following outline. Section 2 reviews background material on "fractal escape-time plots". Section 3 surveys the structure of ionizing trajectories, including the two important results, Facts 1 and 2, concerning patterns among the $(-o)$-strings. Section 4 states the symbolic algorithm for generating $(-o)$-strings, and Appendix A provides the justification for the algorithm. Appendices B and C prove Facts 1 and 2, respectively.

2 The Dynamical System and the Continuous- and Discrete-Escape-Time Plots

We consider the classical dynamics of the electron in a hydrogen atom that is placed in parallel electric and magnetic fields. Following the detailed discussion in Ref. [2], this system can be appropriately scaled so that the electron has the following Hamiltonian in cylindrical coordinates (ρ, z),

$$H(\rho, z, p_\rho, p_z) = \frac{1}{2}(p_\rho^2 + p_z^2) - \frac{1}{\sqrt{\rho^2 + z^2}} + z + \frac{1}{8}B^2\rho^2 = E, \qquad (1)$$

where B is the scaled magnetic field strength, E is the scaled energy, and the z component of angular momentum is zero. (The electric field strength does not appear explicitly due to the choice of scaling.) For all data in this paper, $B = 4.5$ and $E = -1.3$. The applied fields point in the positive z direction, and hence ionizing trajectories eventually escape in the negative z direction. For our calculations, the detector is placed at $z = -4$ [6].

The trajectories that form a given pulse all come from a particular interval of the initial outgoing angle θ, defined as the angle between the initial momentum and the positive z-axis [7]. This is evident from a plot of the time t that it

Fig. 2. (a) The continuous-escape-time plot: the time t for a trajectory launched from the nucleus at angle θ to reach the detector at $z = -4$. Note that time increases *downward* along the vertical axis. (b) The discrete-escape-time plot: the number of iterates of a map required for the electron to escape. (c) An enlargement of an interval in (b).

takes a trajectory to reach the detector as a function of θ, where we assume that all trajectories have the same energy E and the same initial launch time. Such an *escape-time plot* is shown in Fig. 2(a).

The escape-time plot is divided into smooth regions that look like upside-down *icicles* [8]. On the left and right edge of each icicle, the escape time goes to infinity, and in the middle, it has a minimum. Since most trajectories within an icicle strike the detector shortly after this minimum, each icicle produces a pulse with a large initial flux followed by a decaying tail. Thus, there is a one-to-one correspondence between icicles and pulses, and so we can understand the structure of the pulse train by understanding the structure of the escape-time plot.

In Fig. 2(b), we show a discrete-escape-time plot, which simplifies the continuous-escape-time plot by compressing each icicle into a single *escape segment*, with a constant integer value. Figures 2(a) and 2(b) have been placed end to end to emphasize this connection. The precise definition of the discrete plot involves representing the electron dynamics by a discrete-time Poincaré map. The discrete escape time is then defined as the number of iterates of this map required for the electron to escape a particular region of phase space. This is defined explicitly in Sect. A.1 and in earlier references [1,2].

On the far right of Figs. 2(a) and 2(b) is an interval of θ labeled "Direct". This interval extends all the way to $\theta = \pi$. Trajectories launched at values of θ within this segment escape more or less directly downhill, as discussed in Sect. 3 below. Trajectories from other segments in Fig. 2(b) can be much more complicated. Before considering these trajectories in more detail (Sect. 3), we examine the structure of segments within the escape-time plot itself, following Refs. [9,4].

The escape-time plot exhibits regular repeated structure. In particular, regular infinite sequences of escape segments occur throughout the escape-time plot on all scales. We call these sequences *epistrophes* [10]. They have the following properties: (1) An epistrophe is an infinite sequence of consecutive escape segments that converges geometrically upon the endpoint of another escape segment. (2) An epistrophe converges upon each endpoint of every escape segment (except, of course, for the $\theta = \pi$ endpoint of the direct segment). We therefore say that each escape segment "spawns" two new epistrophes, one on either side. (3) The asymptotic tails of any two epistrophes only differ by a change of scale. These results were proved in an Epistrophe Theorem in

Ref. [9].

In the discrete-escape-time plot, the segments labeled A1, A2, and A3 form the first three segments of an epistrophe that converges on the left endpoint of the direct segment. Similarly, the segments B1 and B2 are the first two segments in a B epistrophe, which converges on the left endpoint of the A1 segment. Likewise, a C epistrophe converges on the right endpoint of the A1 segment. Within the resolution limits of Fig. 2, we see that an epistrophe converges upon each endpoint of every escape segment.

In many cases, new epistrophes are spawned in a regular manner. Note that the B and C epistrophes are spawned exactly two iterates after the A1 segment. The same is true of the D and E epistrophes relative to the A2 segment, as shown in Fig. 2(c). This pattern is repeated throughout the escape-time plot. In Ref. [4] we proved a general rule, called the Epistrophe Start Rule, for such escape-time plots. This rule states that: (1) there is a *minimal set* of escape segments, which is determined by the topological structure of the underlying homoclinic tangle; (2) each segment within the minimal set spawns two new epistrophes some number of iterates $D + 1$ later. (In Fig. 2, $D = 1$.) The integer D is called the *minimum delay time*. (It is a topological parameter of the homoclinic tangle, as discussed in Sect. A.1.)

The Epistrophe Start Rule implies a recursive self-similar structure to the escape-time plot. Each segment in the A epistrophe spawns two new epistrophes after two iterates. Each segment within these new epistrophes also spawns two new epistrophes after two iterates, and so forth. This regular structure accounts for most of the early escape segments. On the other hand, a few segments in Fig. 2 do not fit within this recursive structure. For example, the segment marked by $*$ is not generated by the Epistrophe Start Rule. Similarly, where we would expect to see the G1 segment in Fig. 2(c) we find three distinct escape segments, denoted G1′, G1″, G1‴ [11]. In summary, the Epistrophe Start Rule recursively generates a minimal set of escape segments, but there are typically additional segments occurring in the true escape-time plot. We sometimes call the additional escape segments "strophes" [12]. For important earlier work on fractal escape-time plots and other related functions see Refs. [8,13].

All of the results in this paper apply to the chosen parameters $E = -1.3$, $B = 4.5$, and they describe the entire minimal set of escape segments for this case. As these parameters are varied, the structure of the escape-time plot changes. For example, "strophe" segments may appear or disappear, and more importantly, the value of the minimum delay time D in the Epistrophe Start Rule may change. Our methods can be extended to the case $D > 1$, but for simplicity we restrict consideration in this paper to $D = 1$.

Fig. 3. Ionizing trajectories from the direct escape segment are plotted for a selection of launch angles θ. In the upper left panel, the trajectory launched at $\theta = \pi$ proceeds from the nucleus directly downward. This panel also shows potential contours, with the Coulomb center at the origin and the potential saddle at $z = -1$. The unstable periodic orbit near the saddle appears as a thick shaded horizontal line. In the remaining panels, the launch angle θ approaches the critical angle of the direct segment, and the resulting trajectories exhibit an increasing amount of oscillation along the periodic orbit.

3 Description of the structure of ionizing trajectories

We examine the structure of ionizing electron trajectories in the coordinates ρ, z. These trajectories move on the potential surface illustrated by the contours in Fig. 3. This surface has an infinite Coulomb well with a saddle separating the well from the escape channel. Trajectories begin at the nucleus, oscillate chaotically within the Coulomb well, and eventually pass over an unstable orbit which lies near the saddle. This unstable orbit is shown as the thick shaded horizontal line in Fig. 3.

The trajectories that form the direct segment have the simplest behavior (Fig. 3). The trajectory launched at $\theta = \pi$ proceeds directly downhill and reaches the detector first. Adjusting θ away from π, the trajectory oscillates in ρ as it travels down toward the detector. As θ approaches the critical angle at the edge of the escape segment, the frequency of ρ oscillations near the saddle is nearly constant, but the z velocity near the saddle grows smaller and smaller. As a result, for trajectories launched near the critical angle, the ρ oscillations accumulate along the unstable periodic orbit as the trajectory passes over the saddle region. At the critical angle itself, the trajectory oscillates forever, converging upon the periodic orbit.

The trajectories forming the A1 segment exhibit a qualitatively different behavior. Figure 4 shows the trajectory from the A1 icicle that reaches the detector first, with $\theta = 2.04293$. It initially moves downward, away from the nucleus, then passes under and around the nucleus, and finally escapes. As it travels farther downward, toward the detector, it continues to oscillate in ρ. Adjusting the launch angle away from $\theta = 2.0428$, the ionizing trajectory still displays the same qualitative initial behavior, but as it passes over the saddle region on its way toward the detector, it undergoes an increasing number of ρ oscillations close to the unstable periodic orbit, analogous to the direct trajectories in Fig. 3. This is a general phenomenon: All trajectories within a given escape segment display the same initial qualitative behavior but differ in the amount of ρ oscillation as they move past the saddle toward the detector. Thus, to understand the qualitative behavior of the ionizing trajectories within a given segment, we concentrate on a single representative trajectory, taken to be the trajectory that strikes the detector first. Figure 4 plots an

Fig. 4. The earliest trajectory from various pulses, or escape segments, is shown. The electric and magnetic fields point along the z-axis, which is the vertical axis. The segment label, $(-o)$-string, and launch angle θ are shown in each panel. The thick shaded horizontal line is the same periodic orbit shown in Fig. 3.

assortment of such trajectories.

Let us examine the trajectories within the A epistrophe. As with the $\mathsf{A1}$ trajectory, the $\mathsf{A2}$ trajectory initially moves downward and passes under the nucleus. However, it undergoes an additional half-cycle in ρ before looping around the nucleus and exiting [14]. Similarly, the $\mathsf{A3}$ and $\mathsf{A4}$ trajectories oscillate one additional half-cycle each before encircling the nucleus. This pattern persists as one progresses through the A epistrophe: trajectories from consecutive escape segments oscillate one additional half-cycle before encircling the nucleus and escaping. These additional oscillations are close to the unstable periodic orbit, converging upon it as one progresses deeper into the epistrophe.

As stated in the Introduction, we record this qualitative behavior by a finite string of the symbols $\{-, o\}$. (This $(-o)$-string is the same for all trajectories within an escape segment.) Each time a trajectory intersects the negative z-axis, we record the symbol o if the trajectory has encircled the nucleus since its last intersection. If it has not encircled the nucleus, we record the symbol $-$. We record the symbols from left to right, beginning with the first intersection away from the nucleus and ending when the trajectory encircles the nucleus for the last time. For example, the A1, A2, A3, and A4 trajectories yield strings $-o$, $--o$, $---o$, and $----o$, respectively. More generally, we will see that an $\mathsf{A}k$ trajectory yields $-^k o$, where $-^k$ is shorthand for a string of k dashes.

Considering now the B epistrophe, the $\mathsf{B1}$ – $\mathsf{B4}$ trajectories have strings $-o-o$, $-o--o$, $-o---o$, and $-o----o$, respectively (Fig. 4). As with the A epistrophe, successive trajectories oscillate one additional half-cycle in ρ before their last loop around the nucleus. More generally, we will see that the $\mathsf{B}k$ trajectory yields $(-o)-^k o$. The parentheses highlight the fact that the "prefix" $(-o)$ of the string is equal to the string of the $\mathsf{A1}$ segment, which spawns the B epistrophe.

Considering the C epistrophe, we find the same situation, with one striking exception. Figure 4 shows that trajectories $\mathsf{C2}$ – $\mathsf{C4}$ follow the pattern $(-o)-^k o$ (as do all $\mathsf{C}k$ for $k > 1$), but the $\mathsf{C1}$ trajectory breaks this pattern, yielding $--oo$. The difference between the true $(-o)$-string $--oo$ and the "expected" string $-o-o$ is a transposition of the second and third symbols, reflected in Fig. 4 by the fact that the C1 trajectory first encircles the nucleus counterclockwise rather than clockwise, as all subsequent trajectories Ck do.

Note that some escape segments, such as $\mathsf{B2}$ and $\mathsf{C2}$, have the same $(-o)$-string. Thus the $(-o)$-string is not a unique symbolic labeling, as one typically defines for the logistic map or Smale horseshoe – that is not the purpose of the $(-o)$-string. Its purpose is to qualitatively describe what a trajectory looks like in configuration space.

Next consider the D and E epistrophes, spawned by the $\mathsf{A2}$ segment. Trajectories from $\mathsf{D}k$ display the consistent pattern $(- - o) -^k o$ for $k \geq 1$, as seen for $\mathsf{D1}$ – $\mathsf{D4}$ in Fig. 4. Here, the prefix $(- - o)$ equals the string of the spawning segment $\mathsf{A2}$. Trajectories from the E epistrophe, however, only display this pattern for $k \geq 3$. As with $\mathsf{C1}$, the $\mathsf{E1}$ and $\mathsf{E2}$ trajectories break the pattern.

The F and G epistrophes are expected to display the pattern $(- - oo) -^k o$, since they both converge upon $\mathsf{C1}$, which has the string $- - oo$. The $\mathsf{F1}$ segment is the only one to break this pattern.

In the G epistrophe, the Epistrophe Start Rule forces they existence of one segment $\mathsf{G1}$, but two additional segments are observed in Fig. 2c, resulting in the three segments $\mathsf{G1}'$, $\mathsf{G1}''$, and $\mathsf{G1}'''$. All three segments exhibit the same string $(- - oo) - o$.

Finally, the segment marked $*$, which is not a member of the minimal set and which is the first segment to break the regular recursive structure of the escape-time plot, has the string $-oo-o$. This string is different from any string within the minimal set. We shall say nothing more about such strings in this paper.

The trajectories considered above illustrate the following general facts, which are valid within the minimal set.

Fact 1 *A trajectory from a segment within an epistrophe encircles the nucleus once more than a trajectory from the segment spawning the epistrophe. That is, an epistrophe segment yields a string with one more o than the spawning segment.*

Fact 2 *A trajectory from a segment $\mathsf{X}k$ within an epistrophe yields the string $P -^k o$, for $k \geq k_0$, where P is the $(-o)$-string of the segment Y that spawned the epistrophe and where k_0 is the index of the first segment to follow the pattern $P -^k o$. (Hence, once the pattern is realized, all successive trajectories must also follow the pattern.) Furthermore, $k_0 \leq n$, where n is the iterate of the spawning segment Y.*

Fact 2 is a manifestation of continuity in the dynamics: as segments $\mathsf{X}k$ of an arbitrary epistrophe converge upon the spawning segment Y, the initial behavior of a trajectory in $\mathsf{X}k$ converges to the initial behavior of the trajectory at the edge of Y.

In the next section, we present an algebraic process that predicts the qualitative structure of ionizing trajectories. Specifically, we give a symbolic algorithm that computes the $(-o)$-string for any segment in the minimal set, thereby describing the sequence of crossings of the negative z-axis and loops around the nucleus. This algorithm correctly describes the behavior of all the trajectories shown in Fig. 4, except the trajectory $*$ which is not in the minimal set. It also implies Facts 1 and 2 (proved in Appendices B and C), and it correctly predicts the structure of the seemingly exceptional cases like C1, E1 and E2.

4 Algorithm for determining the $(-o)$-string of an escape segment

Now we present the algorithm for computing the string of symbols $\{-, o\}$ for any segment within the minimal set. The algorithm uses an extension of a type of symbolic dynamics that we previously developed to prove the existence and structure of the minimal set of escape segments [4]. However the algorithm itself is self-contained – it can be applied with no knowledge of the underlying meaning of the symbols. The meaning of the symbols and the justification of the algorithm are given in Appendix A.

4.1 Generating the minimal set

We present a symbolic scheme to construct the minimal set of escape segments in the discrete-escape-time plot. First, we introduce an infinite set of symbols

$$\begin{aligned} A =&\{h_0, h_1, c_1, F, \tilde{F}, u_0, u_1, u_2, ..., \\ &h_0^{-1}, h_1^{-1}, c_1^{-1}, F^{-1}, \tilde{F}^{-1}, u_0^{-1}, u_1^{-1}, u_2^{-1}, ...\}, \end{aligned} \tag{2}$$

where each symbol has an inverse. We then introduce a map $\mathcal{M}$ that takes any symbol to a product of symbols

$$\mathcal{M}(h_0) = h_1, \tag{3a}$$
$$\mathcal{M}(h_1) = h_0 u_0^{-1} F, \tag{3b}$$
$$\mathcal{M}(c_1) = \tilde{F}^{-1} u_0^{-1} F, \tag{3c}$$
$$\mathcal{M}(F) = \mathcal{M}(\tilde{F}) = c_1^{-1} u_0^{-1} F, \tag{3d}$$
$$\mathcal{M}(u_n) = u_{n+1}, \qquad 0 \leq n. \tag{3e}$$

The iterate of the inverse of a symbol follows standard convention, e.g. $\mathcal{M}(h_1^{-1}) = F^{-1} u_0 h_0^{-1}$, and the iterate of a product is the product of the iterates. Beginning with $\ell_0 = h_0$, we repeatedly apply Eqs. (3) to map ℓ_n forward to ℓ_{n+1}. For example, the first four iterates are

$$\ell_0 = h_0, \tag{4a}$$
$$\ell_1 = h_1, \tag{4b}$$
$$\ell_2 = h_0 u_0^{-1} F, \tag{4c}$$
$$\ell_3 = h_1 u_1^{-1} c_1^{-1} u_0^{-1} F, \tag{4d}$$
$$\ell_4 = h_0 u_0^{-1} F u_2^{-1} F^{-1} u_0 \tilde{F} u_1^{-1} c_1^{-1} u_0^{-1} F. \tag{4e}$$

The structure of the minimal set of escape segments up to iterate N is encoded in the product ℓ_N. Specifically, each $u_0^{\pm 1}$ factor in ℓ_N corresponds to a segment that escapes at iterate N. More generally, the entire minimal set up to iterate N is obtained from the following rules:

(1) Each $u_n^{\pm 1}$ symbol in ℓ_N corresponds to a segment that escapes in $N - n$ iterates.
(2) The relative positions of the $u_n^{\pm 1}$ symbols in ℓ_N are the same as the relative positions of their corresponding escape segments along the θ-axis, with symbols further to the left corresponding to segments at smaller θ.

This algebraic scheme is a modification of the symbolic dynamics developed in Ref. [4]. There we showed how the symbolic dynamics results in the epistrophe structure, including the Epistrophe Start Rule.

The rest of the algorithm constructs the $(-o)$-string associated with each segment (i.e. each $u_n^{\pm 1}$) within ℓ_N.

4.2 The A-string and 01*-string of an escape segment*

We label each escape segment in the minimal set by a unique string of symbols from the alphabet A. To this end, we recognize that each $u_0^{\pm 1}$ symbol within a given ℓ_n results from mapping forward a symbol s_{n-1} within ℓ_{n-1}, which in turn results from a symbol s_{n-2} within ℓ_{n-2}, and so forth. Thus, each $u_0^{\pm 1}$ within ℓ_n is uniquely identified by a string of "ancestors" $s_1 ... s_{n-1} u_0$, which we call the ancestry string, or A-string, of the segment [to distinguish it from the $(-o)$-string.] Omitting the common ancestor $s_0 = h_0$, we begin the A-string at $s_1 = h_1$ and end it at $s_n = u_0$. Furthermore, we do not record the exponent ± 1 of a symbol in the A-string.

As examples, we determine the A-strings of the A1, A2, and A3 segments in Fig. 2. We first note that these are the rightmost segments at iterates 2, 3, and 4, respectively, meaning that they correspond to the rightmost u_0-factors in Eqs. (4c) – (4e). Then, tracing the ancestry of each of these factors yields the A-strings $h_1 u_0$, $h_1 F u_0$, and $h_1 F F u_0$, respectively. Table 1 shows the A-strings for a selection of escape segments.

Table 1
The A-strings, 01-strings, and $(-o)$-strings for a selection of escape segments.

Segment	A-string	01-string	$(-o)$-string
A1	h_1u_0	$1u$	$-\ o$
A2	h_1Fu_0	$10u$	$--\ o$
A3	h_1FFu_0	$100u$	$---o$
A$k, k \geq 1$	$h_1F^{k-1}u_0$	$10^{k-1}u$	$-^k o$
B1	$h_1h_0h_1u_0$	$111u$	$-o-o$
B2	$h_1h_0h_1Fu_0$	$1110u$	$-o--o$
B3	$h_1h_0h_1FFu_0$	$11100u$	$-o---o$
B$k, k \geq 1$	$h_1h_0h_1F^{k-1}u_0$	$1110^{k-1}u$	$(-o)\ -^k\ o$
C1	$h_1Fc_1u_0$	$101u$	$--oo$
C2	$h_1Fc_1Fu_0$	$1010u$	$-o--o$
C3	$h_1Fc_1FFu_0$	$10100u$	$-o---o$
C$k, k \geq 2$	$h_1Fc_1F^{k-1}u_0$	$1010^{k-1}u$	$(-o)\ -^k\ o$
D1	$h_1Fc_1\tilde{F}u_0$	$1011u$	$--o-o$
D2	$h_1Fc_1\tilde{F}Fu_0$	$10110u$	$--o--o$
D3	$h_1Fc_1\tilde{F}FFu_0$	$101100u$	$--o---o$
D$k, k \geq 1$	$h_1Fc_1\tilde{F}F^{k-1}u_0$	$10110^{k-1}u$	$(--o)\ -^k\ o$
E1	$h_1FFc_1u_0$	$1001u$	$---oo$
E2	$h_1FFc_1Fu_0$	$10010u$	$---o-o$
E3	$h_1FFc_1FFu_0$	$100100u$	$--o---o$
E$k, k \geq 3$	$h_1FFc_1F^{k-1}u_0$	$10010^{k-1}u$	$(--o)\ -^k\ o$
F1	$h_1Fc_1Fc_1u_0$	$10101u$	$-o--oo$
F2	$h_1Fc_1Fc_1Fu_0$	$101010u$	$--oo--o$
F3	$h_1Fc_1Fc_1FFu_0$	$1010100u$	$--oo---o$
F$k, k \geq 2$	$h_1Fc_1Fc_1F^{k-1}u_0$	$101010^{k-1}u$	$(--oo)\ -^k\ o$
G1	$h_1Fc_1\tilde{F}c_1u_0$	$10111u$	$--oo-o$
G2	$h_1Fc_1\tilde{F}c_1Fu_0$	$101110u$	$--oo--o$
G3	$h_1Fc_1\tilde{F}c_1FFu_0$	$1011100u$	$--oo---o$
G$k, k \geq 1$	$h_1Fc_1\tilde{F}c_1F^{k-1}u_0$	$101110^{k-1}u$	$(--oo)\ -^k\ o$

We simplify a given A-string to a string of symbols $\{0, 1, u\}$ using the following identifications, denoted by Σ,

$$\Sigma(h_0) = \Sigma(h_1) = \Sigma(c_1) = \Sigma(\tilde{F}) = 1, \tag{5a}$$

$$\Sigma(F) = 0, \tag{5b}$$

$$\Sigma(u_0) = u. \tag{5c}$$

We call the result a 01-string, read as either "zero-one string" or "naught-one string". Table 1 shows the 01-strings for various escape segments. It is not difficult to show that Eqs. (3) permit a unique reconstruction of the A-string from its corresponding 01-string. Thus, both the A-string and the 01-string label a unique escape segment in the minimal set [unlike the $(-o)$-string.]

4.3 Computing the $(-o)$-string

From the 01-string $S = s_1 ... s_n$ of an escape segment, we can compute the $(-o)$-string. Each symbol s_i of S is mapped to either o or $-$ according to the following:

Translation Rules

(1) First, S begins with a string of 1's whose length m is odd. This string 1...1 maps to the alternating sequence $-o - o ... -$ of length m.

(2) Each 0 within a substring 0...0 maps to $-$, except for the final 0, which can map to either $-$ or o, as determined by Rule 3 or 4.

(3) The symbol u translates to o. Furthermore, the substring $0u$ translates to $-o$.

(4) Any substring 01...1 is analyzed as follows (assuming this substring is maximal, i.e. the next symbol is not 1.) First, break the string into consecutive pairs:

[01][11]...[11]	if length is even,
[01][11]...[11]1	if length is odd.

The terminal *unpaired* 1, which occurs for odd length, maps to $-$. Each pair $[s_\kappa 1]$ maps to either $-o$ or $o-$ according to the "Pair Test" below. Here, κ is the position of the first symbol of the pair within the entire string S.

Pair Test

(a) Construct the infinite periodic sequence $\bar{Q} = QQ...$, where $Q = s_1 ... s_\kappa 1 s_\kappa ... s_2$. Denote the symbols within $\bar{Q}$ by q_i, i.e. $\bar{Q} = q_1 q_2 ...$.

(b) Let λ be the first index where S and $\bar{Q}$ disagree, i.e. $\lambda = \min\{i | s_i \neq q_i\}$.

(c) Let α be the number of 1's within the substring $q_{\kappa+1} ... q_\lambda$ of $\bar{Q}$.

(d) Then,

$$s_\kappa 1 \text{ translates to } \begin{cases} o- \text{ if } \alpha \text{ is even,} \\ -o \text{ if } \alpha \text{ is odd.} \end{cases}$$

4.4 Examples

The rules for translating a 01-string into a $(-o)$-string are best understood through examples. We apply these rules, from left to right, on several 01-strings from Table 1.

A1: Considering the string $1u$, 1 maps to $-$ according to Rule 1, and u maps to o according to Rule 3.

A2: Considering $10u$, 1 maps to $-$ (Rule 1) and $0u$ maps to $-o$ (Rule 3).

A3: Considering $100u$, 1 maps to $-$ (Rule 1), 0 maps to $-$ (Rule 2), and $0u$ maps to $-o$ (Rule 3).

A4: Considering $1000u$, 1 maps to $-$ (Rule 1), 00 maps to $--$ (Rule 2), and $0u$ maps to $-o$ (Rule 3).

B1: Considering $111u$, 111 maps to $-o-$ (Rule 1), and u maps to o (Rule 3).

B2: Considering $1110u$, 111 maps to $-o-$ (Rule 1), and $0u$ maps to $-o$ (Rule 3).

B3: Considering $11100u$, 111 maps to $-o-$ (Rule 1), 0 maps to $-$ (Rule 2), and $0u$ maps to $-o$ (Rule 3).

C1: Considering $101u$, 1 maps to $-$ (Rule 1). Then, 01 is analyzed according to Rule 4. That is, we apply the Pair Test to 01, for which $\kappa = 2$.

a. $Q = s_1 s_2 1 s_2 = 1010$ and $\bar{Q} = (1010)(1010)...$.
b. Comparing $S = 101u$ to $\bar{Q} = 1010...$, the first difference occurs at $\lambda = 4$.
c. The substring $q_{\kappa+1}...q_\lambda = q_3 q_4$ is 10. Hence $\alpha = 1$.
d. Since α is odd, 01 maps to $-o$.

Finally, u maps to o (Rule 3), and hence $101u$ maps to $- - oo$.

C2: Considering $1010u$, we only describe how to implement Rule 4, having sufficiently illustrated the other rules. The Pair Test applies to 01 with $\kappa = 2$. We skip Step (a) of the Pair Test, since it is identical to Step (a) for C1.

b. Comparing $S = 1010u$ to $\bar{Q} = 101010...$, $\lambda = 5$.

c. $q_{\kappa+1}...q_\lambda = q_3q_4q_5 = 101$. Hence $\alpha = 2$.
d. Since α is even, 01 maps to $o-$.

Here, the Pair Test returns $o-$, the transpose of the result returned for C1. One can verify that the result for C3 is the same as for C2.

A more involved application of the Pair Test occurs for the E epistrophe.

E1: Considering $1001u$, the Pair Test applies to 01 with $\kappa = 3$.

a. $Q = s_1s_2s_31s_3s_2 = 100100$.
b. Comparing $S = 1001u$ to $\bar{Q} = 10010...$, $\lambda = 5$.
c. $q_{\kappa+1}...q_\lambda = q_4q_5 = 10$. Hence $\alpha = 1$.
d. Since α is odd, 01 maps to $-o$.

E2: Considering $10010u$, the Pair Test applies to 01 with $\kappa = 3$. We skip Step (a), since it is identical to that of E1.

b. Comparing $S = 10010u$ to $\bar{Q} = 100100...$, $\lambda = 6$.
c. $q_{\kappa+1}...q_\lambda = q_4q_5q_6 = 100$. Hence $\alpha = 1$.
d. Since α is odd, 01 maps to $-o$.

E3: Considering $100100u$, the Pair Test applies to 01 with $\kappa = 3$. We again skip Step (a).

b. Comparing $S = 100100u$ to $\bar{Q} = 1001001...$, $\lambda = 7$.
c. $q_{\kappa+1}...q_\lambda = q_4q_5q_6q_7 = 1001$. Hence $\alpha = 2$.
d. Since α is even, 01 maps to $o-$.

Notice that for C1, E1, and E2, the Pair Test returns $-o$, but for C2, E3 and all subsequent Ck's and Ek's the test returns $o-$. The Pair Test thus produces both the asymptotic pattern of the epistrophe segments, as well as the initial behavior that breaks the pattern.

G3: The string $S = 1011100u$ requires two applications of the Pair Test. We illustrate this with the following diagram

$$
\begin{array}{lllllllllll}
\text{Rule \#} & & 1 & 4 & 4 & 4 & 4 & 2 & 3 & 3 & \\
 & & - & [\,- & o\,] & [\,o & - &]\,- & - & o & \\
 & & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \uparrow & \\
S & = & 1 & [\,0 & 1\,] & [\,1 & 1 &]\,0 & 0 & u & \\
 & & & & & & & & & & \\
\bar{Q}_1 & = (& 1 & 0 & \underline{1} & \underline{0}\,)(& 1 & 0 & 1 & 0 &)... \\
 & & & \kappa_1 & & \lambda_1 & & & & & \\
\bar{Q}_2 & = (& 1 & 0 & 1 & 1 & \underline{1} & \underline{1} & 1 & 0 &)... \\
 & & & & & \kappa_2 & & \lambda_2 & & &
\end{array}
\tag{6}
$$

Here, each symbol of S is connected to its corresponding $\{-, o\}$-symbol by an upward pointing arrow. Above each $\{-, o\}$-symbol is the number of the Translation Rule used. The first three rules are easily applied, and so we concentrate here on the application of the Pair Test to the two pairs, which are set off by square brackets.

The first pair begins at $\kappa_1 = 2$. Directly below S we record $\bar{Q}_1 = Q_1 Q_1 ...$, with each factor $Q_1 = s_1 s_2 1 s_2$ enclosed in parentheses. The first three symbols of $\bar{Q}_1$ and S agree, with the first discrepancy occurring at $\lambda_1 = 4$. The string $q_{\kappa_1+1} ... q_{\lambda_1} = q_3 q_4 = 10$ is underlined for visibility. Since this string contains only one 1, we find $\alpha = 1$ and hence $s_2 1$ translates to $-o$.

For the second pair, which begins at $\kappa_2 = 4$, we record $\bar{Q}_2 = Q_2 Q_2 ...$. The first discrepancy now occurs at $\lambda_2 = 6$, meaning that the string $q_{\kappa_2+1} ... q_{\lambda_2} = q_5 q_6 = 11$ contains two 1's, and hence $\alpha = 2$ and $s_4 1$ translates to $o-$.

The reader is encouraged to work through the remaining examples Dk, Fk, and Gk in Fig. 4 and Table 1. In summary, all the preceding examples illustrate that the algorithm correctly predicts the qualitative structure of the ionizing trajectories that occur within the minimal set of escape segments.

5 Conclusions

In previous work, we predicted that hydrogen atoms in parallel electric and magnetic fields can decay by emitting a train of electron pulses. The ionizing trajectories that form a given pulse lie within a particular interval, or escape segment, of the initial launch angle θ. All trajectories within such an interval exhibit similar qualitative behavior. In the present work, we studied the spatial shapes of these trajectories. In particular, we developed an algorithm, based on symbolic dynamics, whose output is the qualitative shape of trajectories that lie within a certain minimal set of escape segments. Although this algorithm is nontrivial, it has simple consequences, which were summarized by Facts 1 and 2.

Acknowledgements

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A Justification of the Algorithm

We explain here the geometry underlying the algorithm presented in Sect. 4. The algorithm takes essential information about the history of an orbit within a Poincaré surface of section (the A-string) and converts it into information about the orbit in configuration space [the $(-o)$-string]. The structure of the dynamics in the surface of section is described in terms of a homoclinic tangle. For a selection of important work on tangles and phase space transport, see Ref. [15].

A.1 The surface of section and homoclinic tangle

Within the three-dimensional energy shell of the four-dimensional phase space (ρ, z, p_ρ, p_z), we define a two-dimensional Poincaré surface of section consisting of the negative z-axis and its conjugate momentum p_z. More precisely, the surface of section is the constraint surface defined by $H = E$, $\rho = 0$, $z \leq 0$, where the two branches $p_\rho > 0$ and $p_\rho < 0$ are mathematically identified into a single component. We define $\mathcal{M}$ to be the associated Poincaré return map which maps this surface to itself. To regularize the infinite momentum at the Coulomb singularity, we express $\mathcal{M}$ in new canonical coordinates $q = (1 - p_z^2)\sqrt{-z/(1+p_z^2)}$ and $p = -2p_z\sqrt{-z/(1+p_z^2)}$ on the surface of section. Figure A.1 shows the qualitative structure of a surface-of-section plot in these coordinates. For further details see Refs. [1,2].

The prominent unstable periodic orbit, shown as the shaded line in Figs. 3 and 4, intersects the negative z-axis, forming an unstable fixed point $\mathbf{z}_\mathsf{X}$ of the Poincaré map $\mathcal{M}$, as shown in Fig. A.1. This fixed point has stable $(\mathcal{S})$

and unstable ($\mathcal{U}$) manifolds that intersect in a complicated pattern, called a homoclinic tangle.

The intersection of $\mathcal{S}$ and $\mathcal{U}$ at $\mathbf{P}_0$ defines a region of the qp-plane which we call the *complex*. The $\mathcal{S}$- and $\mathcal{U}$-boundaries of the complex are the segments of $\mathcal{S}$ and $\mathcal{U}$ that join $\mathbf{P}_0$ to $\mathbf{z}_{\mathsf{X}}$.

The ensemble of initial states, located at the nucleus and spanning all launch angles θ, forms a line of initial conditions $\mathcal{L}_0$ in the qp-plane. This line is parameterized by θ, beginning at the origin $(q, p) = (0, 0)$, with $\theta = 0$, and continuing horizontally to the left past $\mathbf{P}_0$. (The origin is a fixed point of $\mathcal{M}$.) The discrete escape time is formally defined as the number of iterates of $\mathcal{M}$ required for a point on $\mathcal{L}_0$ to map out of the complex. Once a trajectory escapes the complex, it never returns.

The intersection $\mathbf{P}_0$ maps to an infinite sequence of intersections $\mathbf{P}_n = \mathcal{M}^n(\mathbf{P}_0)$, $-\infty < n < \infty$. Likewise, the intersection $\mathbf{Q}_0$, shown in Fig. A.1, maps to $\mathbf{Q}_n = \mathcal{M}^n(\mathbf{Q}_0)$. These intersections define regions E_n (*escape lobes*) and C_n (*capture lobes*), $-\infty < n < \infty$. The $\mathcal{S}$- and $\mathcal{U}$-boundaries of E_n are the segments of $\mathcal{S}$ and $\mathcal{U}$ that join $\mathbf{P}_n$ to $\mathbf{Q}_n$, whereas the $\mathcal{S}$- and $\mathcal{U}$-boundaries of C_n join $\mathbf{Q}_{n-1}$ to $\mathbf{P}_n$.

Under the Poincaré map, $\mathcal{M}(E_n) = E_{n+1}$ and $\mathcal{M}(C_n) = C_{n+1}$. Thus, the escape lobe E_{-1}, which is inside the complex, maps to E_0, which is outside the complex. In fact, the lobe E_{-1} contains all points that map out of the complex. Similarly, C_0 contains all points that map into the complex.

We describe the topology of the tangle by the minimum delay time D, defined as the smallest n such that C_{n+1} intersects E_0. It is the minimum number of iterates a scattering trajectory may spend inside the complex. In Fig. A.1, $D = 1$. For more details on homoclinic tangles and phase space transport, see Ref. [15].

We approximate the true Poincaré map by a map having the simplest topological structure consistent with $D = 1$. Such a map is topologically equivalent to a Smale horseshoe. This approximation produces only escape segments that are in the minimal set; there are no additional strophe segments. To justify the algorithm for the exact dynamics exhibited by the hydrogen system requires a more detailed mathematical treatment than is appropriate here. The symbol $\mathcal{M}$ will henceforth refer to the approximate map.

Fig. A.1. This figure shows a qualitative picture of the tangle and one representative curve from each class. The unstable manifold $\mathcal{U}$ is the thick curve, and the stable manifold $\mathcal{S}$ is the corresponding thin curve. The capture lobes C_1 and C_2 are shaded dark. The escape lobe E_{-1} is bounded below by $\mathcal{U}$ and above by $\mathcal{S}$; it is the reflection of C_1 through the horizontal axis. The intersection between E_{-1} and C_1 yields the minimum delay time $D = 1$.

A.2 Topological significance of the symbols in A

Each symbol in A [Eq. (2)] represents a class of directed curves in the qp-plane. Only the endpoints of these curves can intersect the $\mathcal{S}$-boundary of the complex. Furthermore, they satisfy (see Fig. A.1):

h_0: Curves go directly from the origin to the $\mathcal{S}$-boundary of E_0, denoted $\mathcal{E}_0$, without intersecting C_1, C_2, or $\mathcal{L}_0$.

h_1: Curves go directly from the origin to the $\mathcal{S}$-boundary of E_1, denoted $\mathcal{E}_1$, without intersecting C_1, C_2, or $\mathcal{L}_0$.

c_1: Curves go from $\mathcal{E}_0$ to $\mathcal{E}_1$, passing between C_1 and the origin and not intersecting $\mathcal{L}_0$.

$\tilde{F}$: Curves go from $\mathcal{E}_0$ to $\mathcal{E}_1$, passing under both C_1 and the origin, intersecting $\mathcal{L}_0$ once, but staying above C_2.

F: Curves go from $\mathcal{E}_0$ to the segment of $\mathcal{S}$ joining $\mathbf{P}_2$ to $\mathbf{z}_\mathsf{X}$, passing under C_2, and intersecting $\mathcal{L}_0$ once.

$u_n, n \geq 0$: Curves stay within E_n, beginning and ending on the $\mathcal{S}$-boundary of E_n, and passing clockwise over $C_{n+2} \cap E_n$.

The inverse a^{-1} of a symbol $a \in A$ is defined as the same class of curves as a, except with the directions reversed. The product ab of two symbols $a, b \in A$, as used in Eqs. (3) and (4), is defined as a new class of directed curves, defined by concatenating a curve in a with a curve in b, such that the last point of a agrees with the first point of b. (Note, however, that juxtaposition of symbols in an A-string does *not* indicate multiplication or concatenation.)

Under the Poincaré map $\mathcal{M}$ on the qp-plane, each class of curves $a \in A$ is mapped to another class of curves, described by a product of elements in A. This mapping is given by Eqs. (3). These equations can be justified by scrutiny of Fig. A.1. (See Ref. [4] for further detail.)

Since the line of initial conditions $\mathcal{L}_0$ intersects C_2, it is not of type h_0, according to the above definition. However, $\mathcal{L}_0$ does map to a curve of type h_1, and for that reason we begin with $\ell_0 = h_0$ in Eqs. (4).

Fig. A.2. (a) The regions D_0 and D_1 (shaded). (b) The regions D'_0 and D'_1, which are the reflections of D_0 and D_1, respectively.

Finally, since u_0 lies within E_0, a $u_0^{\pm 1}$ factor within ℓ_N represents a piece of the curve $\mathcal{L}_N$ that intersects E_0. That is, each $u_0^{\pm 1}$ factor represents a segment that escapes on the Nth iterate.

A.3 Topological significance of the symbols $\{0, 1, u\}$

We define two regions of the complex, D_0 and D_1, as shown in Fig. A.2(a). We define a map Σ that takes a point $\mathbf{z} \in D_0 \cup D_1 \cup E_0$ and returns 0, 1, or u according to

$$\Sigma(\mathbf{z}) = \nu \quad \text{for} \quad \mathbf{z} \in D_\nu, \qquad \nu = 0, 1, \tag{A.1}$$

$$\Sigma(\mathbf{z}) = u \quad \text{for} \quad \mathbf{z} \in E_0. \tag{A.2}$$

Since all symbols in A, except u_n, $n > 0$, label classes of curves that lie entirely within either D_0, D_1, or E_0, the map Σ can be extended to act directly on these symbols, which leads to Eqs. (5).

A.4 A criterion for encircling the nucleus

We imagine interpolating between a point $\mathbf{z}$ and its image $\mathcal{M}(\mathbf{z})$ by a curve that begins at $\mathbf{z}$ and moves clockwise (about the origin) to $\mathcal{M}(\mathbf{z})$. If this clockwise motion crosses $\mathcal{L}_0$, we assert that the corresponding electron trajectory in the ρz-plane encircles the nucleus; and if the clockwise motion does not cross $\mathcal{L}_0$, then the electron does not encircle the nucleus [16]. To be more specific, consider a point in h_1. (We say "a point in h_1" as shorthand for "a point on a curve in the class h_1".) If this point maps clockwise to a point in h_0, it must cross over $\mathcal{L}_0$, and therefore the corresponding electron trajectory encircles the nucleus. Since each appearance of the substring $h_1 h_0$ within an A-string describes a point of the escaping trajectory that maps from h_1 to h_0, this substring translates to τo, with $\tau \in \{-, o\}$ undetermined. The symbol h_0 translates to o because the trajectory encircles the nucleus *before* arriving at the point in h_0, as specified by the conventions for $-$ and o introduced in Sect. 3.

Conversely, a point in h_0 maps clockwise to a point in h_1 without crossing $\mathcal{L}_0$. It therefore does not encircle the nucleus, and each appearance of $h_0 h_1$ in an A-string translates to $\tau-$.

If a point in h_1 maps clockwise to a point in F, it crosses $\mathcal{L}_0$ if and only if it arrives in that piece of F above $\mathcal{L}_0$ (i.e. if it lands between $\mathcal{E}_0$ and $\mathcal{L}_0$.) This piece of F we call F_a, i.e. F_a contains curves that lie between $\mathcal{E}_0$ and $\mathcal{L}_0$. The piece of F below $\mathcal{L}_0$ we call F_b. Then, $h_1 F_a$ translates to τo and $h_1 F_b$ translates to $\tau -$. We apply similar logic to all possible pairs and find:

$$\left.\begin{array}{c} h_1 h_0,\ h_1 u_0,\ h_1 F_a,\ c_1 \tilde{F}_a,\ c_1 u_0,\ c_1 F_a, \\ F_b c_1,\ \tilde{F}_b c_1,\ F_b u_0,\ \tilde{F}_b u_0,\ F_b F_a,\ \tilde{F}_b F_a \end{array}\right\} \to \tau o, \tag{A.3}$$

$$\left.\begin{array}{c} h_0 h_1,\ h_1 F_b,\ c_1 \tilde{F}_b,\ c_1 F_b, \\ F_a c_1,\ \tilde{F}_a c_1,\ F_b F_b,\ \tilde{F}_b F_b \end{array}\right\} \to \tau -, \tag{A.4}$$

where the arrow means "translate to". From Eqs. (A.3) and (A.4), we deduce the following simpler translations

$$F_b,\ \tilde{F}_b \to -, \tag{A.5}$$

$$F_a,\ \tilde{F}_a \to o, \tag{A.6}$$

and

$$h_1 \to -, \tag{A.7}$$

$$h_0,\ u_0 \to o. \tag{A.8}$$

Furthermore, Eqs. (A.3) and (A.4) together with (A.5) and (A.6) yield

$$F_a c_1,\ \tilde{F}_a c_1 \to o-, \tag{A.9}$$

$$F_b c_1,\ \tilde{F}_b c_1 \to -o. \tag{A.10}$$

Notice that $F_a F_a$, $F_a F_b$, $F_a u_0$, $\tilde{F}_a F_a$, $\tilde{F}_a F_b$, and $\tilde{F}_a u_0$ are missing from the list of all possible pairs in Eqs. (A.3) and (A.4). This is because a point in F_a or $\tilde{F}_a$ must map to a point in c_1. This observation, together with Eq. (A.5), implies

$$\left.\begin{array}{c} FF = F_b F \\ \tilde{F}F = \tilde{F}_b F \\ F u_0 = F_b u_0 \\ \tilde{F} u_0 = \tilde{F}_b u_0 \end{array}\right\} \to -\tau. \tag{A.11}$$

Equations (A.7)–(A.11) are sufficient to determine the $(-o)$-string given the A-string, with one stipulation: we must determine whether the F in each substring $F c_1$ is F_a or F_b (and similarly with $\tilde{F} c_1$). This issue is addressed in Sect. A.5, where it is more naturally treated using the 01-string rather than the A-string.

First, we show how the Translation Rules 1 – 4 (except for the Pair Test) follow from Eqs. (A.7)–(A.11).

Rule 1: The initial string 1...1 corresponds to an A-string $h_1 h_0 h_1 h_0 ... h_1$. By Eqs. (A.7) and (A.8), this translates to $-o - o ... -$.

Rule 2: A substring 0...0 corresponds to an A-string $F ... F$. By Eq. (A.11) this maps to a string of $-$'s, except for the final symbol.

Rule 3: By Eq. (A.8), u translates to o. Furthermore, $0u$, which corresponds to Fu_0, translates to $-o$ by Eq. (A.11).

Rule 4: An even substring [01][11]...[11] corresponds to $[Fc_1][\tilde{F}c_1]...[\tilde{F}c_1]$ and an odd substring [01][11]...[11]1 corresponds to $[Fc_1][\tilde{F}c_1]...[\tilde{F}c_1]\tilde{F}$. In the odd case, the terminal 1, which corresponds to $\tilde{F}$, must be followed by either 0, which corresponds to F, or u, which corresponds to u_0. Thus, the terminal $\tilde{F}$ translates to $-$ by Eq. (A.11).

Since each pair [01] corresponds to $[Fc_1]$ and each pair [11] corresponds to $[\tilde{F}c_1]$, these pairs translate to either $o-$ or $-o$ according to Eqs. (A.9) and (A.10). The Pair Test, which resolves this ambiguity, determines on which side of $\mathcal{L}_0$ a point in F lies, i.e. whether the point is in F_a or F_b (and similarly with a point in $\tilde{F}$.)

A.5 Closed orbits

Each F or $\tilde{F}$ factor within ℓ_κ, for some $\kappa > 0$, determines a segment of $\mathcal{L}_\kappa$ that intersects $\mathcal{L}_0$. Since $\mathcal{L}_0$ consists of states at the nucleus, this intersection determines a closed orbit, i.e. a trajectory that begins at, and eventually returns to, the nucleus (after κ iterates.)

Since the dividing point between F_a and F_b is a closed orbit, these orbits warrant further study. In particular, given the first κ symbols in the infinite A-string of a closed orbit, we shall determine the subsequent behavior of the orbit. We describe this behavior using the 01-string.

As a result of time-reversal symmetry, after the first κ iterates of the closed orbit in the qp-plane, $\mathbf{z}_1 ... \mathbf{z}_\kappa$, the orbit retraces its steps, reflected about the q-axis, i.e.

$$\mathbf{z}_{\kappa+i} = R(\mathbf{z}_{\kappa-i}), \quad -\infty < i < \infty, \tag{A.12}$$

where R is the reflection about the q-axis. Thus $\mathbf{z}_{2\kappa} = \mathbf{z}_0$, and hence an orbit that is closed after κ iterates is periodic with period 2κ (though its fundamental period may be less than 2κ.) Consequently, all points $\mathbf{z}_i$ lie inside the complex for $-\infty < i < \infty$.

In addition to the regions D_0 and D_1 in Fig. A.2(a), we define two regions D_0'

and D'_1 in Fig. A.2(b). These regions are related by

$$\mathcal{M}^2(D'_\nu) = D_\nu, \qquad \nu = 0, 1, \tag{A.13}$$
$$R(D_\nu) = D'_\nu, \qquad \nu = 0, 1. \tag{A.14}$$

Analogous to Eq. (A.1), we define

$$\Sigma'(\mathbf{z}) = \mu \text{ for } \mathbf{z} \in D'_\mu, \qquad \mu = 0, 1. \tag{A.15}$$

Then

$$\Sigma'(\mathbf{z}_i) = \Sigma(\mathbf{z}_{i+2}) \tag{A.16}$$

follows immediately from Eqs. (A.1), (A.13), and (A.15), and

$$\Sigma'(\mathbf{z}) = \Sigma(R(\mathbf{z})) \tag{A.17}$$

follows from Eqs. (A.1), (A.14), and (A.15). Combining Eqs. (A.12), (A.16), and (A.17) yields

$$\begin{aligned} \Sigma(\mathbf{z}_{\kappa+1-i}) &= \Sigma'(\mathbf{z}_{\kappa-1-i}) = \Sigma(R(\mathbf{z}_{\kappa-1-i})) \\ &= \Sigma(\mathbf{z}_{\kappa+1+i}). \end{aligned} \tag{A.18}$$

Furthermore, since $\mathcal{L}_0$ maps to a curve of type h_1, we find

$$\Sigma(\mathbf{z}_{\kappa+1}) = 1 \tag{A.19}$$

by Eq. (5a). Thus, denoting the first κ symbols in the 01-string of the trajectory by $s_i = \Sigma(\mathbf{z}_i)$, $i = 1, ..., \kappa$, the first 2κ symbols are

$$Q = s_1 ... s_\kappa 1 s_\kappa ... s_2, \tag{A.20}$$

by Eqs. (A.18) and (A.19). Since the trajectory has period 2κ, its full 01-string is $\bar{Q} = QQ...$.

A.6 Symbol parity

In Sect. 4.2 we defined an A-string to be the list of ancestors for a given u_0 within ℓ_N. These ancestors appear as factors of ℓ_n, $n < N$, as shown in Eqs. (4). Each of these factors has an exponent ± 1 (although this exponent is omitted in the A-string). We call the exponent ± 1 the parity (or sense) of a given symbol. The parity of a symbol in an A-string is naturally inherited by the corresponding symbol in the 01-string. For a given symbol in such a 01-string, how do we recover its parity? The parity of each 1 in the initial string 1...1, which corresponds to $h_0 h_1 ... h_0$, is $+1$ by Eqs. (3a) and (3b). Furthermore,

> For a symbol s_i that is either 0 or a noninitial 1, its parity is $(-1)^{\beta+1}$, where β equals the number of 1's in the substring $s_1 ... s_i$.

This fact follows recursively from Eqs. (3) and the identifications (5): in the 01-string, each new $\tilde{F}$ or c_1 (identified with 1) switches the parity, but each new F (identified with 0) does not.

A.7 An ordering of 01*-strings*

For two 01-strings S and S', we write $S < S'$ if the segment of $\mathcal{L}_0$ specified by S is left of the segment specified by S' in Fig. 2, i.e. S is at smaller launch angle θ than S'. This order can be determined directly from S and S'. To this end, let λ be the first index where S and S' differ, i.e.

$$S = s_1 ... s_{\lambda-1} s_\lambda ..., \tag{A.21}$$
$$S' = s_1 ... s_{\lambda-1} s'_\lambda ..., \tag{A.22}$$

with $s_\lambda \neq s'_\lambda$. If $s_{\lambda-1}$ has parity $+1$, then the order of S and S' is determined solely by the order of s_λ and s'_λ, using the relations $1 < u < 0$. If $s_{\lambda-1}$ has parity -1, then the relations $1 > u > 0$ are used instead. This result follows from interpreting the right hand side of Eqs. (3) in terms of the identifications (5).

A.8 Comparing an escaping orbit to a closed orbit

We can now resolve the ambiguity of a pair $[s_\kappa 1]$ within the 01-string $S = s_1 ... s_{\kappa-1} [s_\kappa 1] s_{\kappa+2} ... u$ of an escaping orbit. We assume for definiteness that $[s_\kappa 1]$ corresponds to $[F c_1]$. (The following argument still applies if it corresponds to $[\tilde{F} c_1]$ instead.) We construct the string $\bar{Q} = QQ...$ [with Q given by Eq. (A.20)] which describes the closed orbit that separates F_a from F_b within the segment F, which corresponds to s_κ. Now, if

$$\begin{array}{l}(S < \bar{Q} \text{ and } s_\kappa \text{ has parity } +1) \text{ or} \\ (S > \bar{Q} \text{ and } s_\kappa \text{ has parity } -1),\end{array} \tag{A.23}$$

then $[s_\kappa 1]$ corresponds to $[F_a c_1]$, which translates to $o-$ by Eq. (A.9). However, if

$$\begin{array}{l}(S < \bar{Q} \text{ and } s_\kappa \text{ has parity } -1) \text{ or} \\ (S > \bar{Q} \text{ and } s_\kappa \text{ has parity } +1),\end{array} \tag{A.24}$$

then $[s_\kappa 1]$ corresponds to $[F_b c_1]$, which translates to $-o$ by Eq. (A.10).

Combining the ordering analysis of Sect. A.7 with the parity test in Sect. A.6, we find that the two cases (A.23) and (A.24) are distinguished simply by the parity of α, defined as the number of 1's within the substring $q_{\kappa+1} ... q_\lambda$, where

λ is the first index where S and $\bar{Q}$ differ. Case (A.23) is α even and case (A.24) is α odd. Thus we have justified the Pair Test. This completes the justification of the rules for translating a 01-string into a $(-o)$-string.

B Proof of Fact 1

An arbitrary segment in the minimal set, whose A-string we denote $\hat{S} = \hat{B}u_0$, spawns an epistrophe on either side. Here, $\hat{B}$ denotes all A-symbols of $\hat{S}$ except for the final u_0. Equations (3) imply that on one side, the epistrophe segments have the form $\hat{B}Fc_1F^{k-1}u_0$, whereas on the other side, they have the form $\hat{B}abF^{k-1}u_0$, where ab is either h_0h_1, $\tilde{F}c_1$, or $c_1\tilde{F}$. As a result, a segment with 01-string $S = Bu$, of total length n, spawns epistrophes of the form

$$R_k = r_1...r_{n+k+1} = Br_n10^{k-1}u, \tag{B.1}$$

where $r_n = 0$ on one side and $r_n = 1$ on the other. Here, a hat above S or B distinguishes an A-string from a 01-string.

We now prove Fact 1 of Sect. 3. There is an easy technique to compute the total number of o's produced by a given 01-string: by Translation Rule 1, the initial string 1...1 of odd length m contributes $\lfloor(m/2)$ o's, where the floor function $\lfloor$ rounds down to the nearest integer; similarly, by Rule 4, each maximal string 01...1 of length m also contributes $\lfloor(m/2)$ o's; finally, by Rule 3, u contributes one o.

We use the above technique to compare the string B within Bu to the string Br_n1 within $Br_n10^{k-1}u$ and show that the latter has one more o. If $r_n = 0$, then any maximal string of 1's within Bu is also maximal within $B01$ and thus has the same value of m, meaning that it produces the same number of o's regardless of whether it is a substring of Bu or $B01$. Hence, the substring 01 within $B01$ produces one extra o total. We leave the analysis of the case $r_n = 1$ to the reader. (Hint: consider the two subcases $r_{n-1} = 0$ and $r_{n-1} = 1$ separately.)

C Proof of Fact 2

Fact 2 is a corollary of

Theorem 1 *Let R_k label the kth segment in an epistrophe spawned by a segment S, which itself occurs at iterate n. Then the first m $\{-, o\}$-symbols generated by S agree with the first m symbols generated by R_k, for all $m \leq n$*

and for all $k \geq k_0(m)$. Here, $k_0(m)$ is the first index at which this agreement occurs. It satisfies $k_0(m) \leq m$. Furthermore, R_k translates to a $(-o)$-string ending in $o -^k o$ for all $k \geq k_0(n)$.

Proof of Theorem 1: From Eq. (B.1), we recall that a segment $S = s_1...s_n = Bu$, of total length n, spawns two epistrophes whose segments have the form $R_k = r_1...r_{n+k+1} = Br_n 10^{k-1}u$, with $k \geq 1$ and $r_n = 0$ on one side and $r_n = 1$ on the other. The 01-strings S and R_k are converted into $(-o)$-strings, denoted here by $\Upsilon(S)$ and $\Upsilon(R_k)$, using the Translation Rules of Sect. 4.3.

We first analyze the initial $n - 1$ symbols of R_k and S. Since these strings are identical, i.e. $s_1...s_{n-1} = r_1...r_{n-1}$, they translate to identical $(-o)$-strings except for the following three conceivable cases:

1. Under the Pair Test, a pair $[s_\kappa 1]$, $\kappa < n - 1$, within S could yield a different $(-o)$-string than $[s_\kappa 1]$ within R_k.
2. $s_{n-1}s_n = 0u$ within S translates to $-o$ (Rule 3). However, $r_{n-1}r_n = 01$ within R_k might translate to $o-$ under the Pair Test.
3. $s_{n-1}s_n = 1u$ within S translates to $-o$ if $s_{n-1} = 1$ is unpaired (as described in Rule 4). However, $r_{n-1}r_n = 11$ within R_k might then translate to $o-$ under the Pair Test.

We discover below that Cases 2 and 3 are in fact forbidden. We address Case 1 with

Lemma 1 *Any pair $[s_\kappa 1]$, $\kappa < n - 1$, within S translates to the same $(-o)$-string as the corresponding pair $[s_\kappa 1]$ within R_k, for $k \geq k_0$. Here, k_0 is the first index of R_k at which this agreement occurs, and it satisfies $k_0 \leq \kappa < n-1$.*

Proof of Lemma 1: Let a pair $[s_\kappa 1]$, $\kappa < n - 1$, of S be given. The equality of the first $n - 1$ symbols of S and R_k guarantees that Step (a) of the Pair Test returns the same Q for both S and R_k. For Step (b), let $\lambda \leq \text{length}(S) = n$ and $\lambda' \leq \text{length}(R_k) = n + k + 1$ be the first indices where S and R_k differ from $\bar{Q}$, respectively. Then, Steps (c) and (d) of the Pair Test imply

Lemma 2 *The Pair Test yields different results for S and R_k if and only if $\Delta\alpha = \alpha' - \alpha$ is odd, where $\Delta\alpha$ equals the number of 1's in the substring $q_{\lambda+1}...q_{\lambda'}$ of $\bar{Q}$.*

When can $\Delta\alpha$ be odd? This is addressed by

Lemma 3 *If $\Delta\alpha$ is odd, then $\lambda = n$ and $\lambda' = n + k + 1$.*

To prove Lemma 3, we first note that $\Delta\alpha$ odd implies $\lambda < \lambda'$, which implies $\lambda = n$ and $n < \lambda' \leq n + k + 1$.

Suppose $\lambda = n$ and $\lambda' = n+1$. Then since $r_{n+1} = 1$ in R_k, the definition of λ' implies $q_{\lambda'} = q_{n+1} = 0$ in $\bar{Q}$. Hence, $q_{\lambda+1}...q_{\lambda'} = q_{n+1} = 0$ and so $\Delta\alpha = 0$. Thus, $\Delta\alpha$ odd implies $\lambda = n$ and $n+1 < \lambda' \leq n+k+1$.

Suppose $\lambda = n$ and $n+1 < \lambda' < n+k+1$. The definition of λ' implies $\bar{Q}$ agrees with R_k for all indices $i < \lambda'$ and differs at $i = \lambda'$. Hence, Eq. (B.1) implies $q_{\lambda+1}...q_{\lambda'} = q_{n+1}...q_{\lambda'} = 10^{\lambda'-n-2}1$, and thus $\Delta\alpha = 2$. This completes the proof of Lemma 3.

We now show that if $[s_\kappa 1]$ yields the same $(-o)$-string within $\Upsilon(S)$ as within $\Upsilon(R_k)$, for some k, then it does for $k+1$ as well. Let k be given such that these $(-o)$-strings agree. If $\lambda' \leq n+1$, then by Lemmas 2 and 3, $[s_\kappa 1]$ in S translates to the same $(-o)$-string as $[s_\kappa 1]$ in R_k, for all $k \geq 1$. We thus need only consider the case $\lambda' > n+1$ and $\lambda = n$. Since Lemma 2 implies $\Delta\alpha$ even, $q_{n+1}...q_{\lambda'}$ must have an even number of 1's. Since $q_{n+1} = r_{n+1} = 1$, there must be a second 1 within $q_{n+2}...q_{\lambda'}$, which can only be $q_{\lambda'} = 1$. Given the form of R_k in Eq. (B.1), the value of λ' is the same for $[s_\kappa 1]$ within R_k as for $[s_\kappa 1]$ within R_{k+1}. Hence, $\Delta\alpha$ is also even for $[s_\kappa 1]$ within R_{k+1}, and by Lemma 2, $[s_\kappa 1]$ yields the same $(-o)$-string within $\Upsilon(R_{k+1})$ as within $\Upsilon(S)$.

We now show $k_0 \leq \kappa$, for which we need only prove that $[s_\kappa 1]$ yields the same $(-o)$-string within both $\Upsilon(S)$ and $\Upsilon(R_\kappa)$. If $\lambda' \neq n+\kappa+1$, then Lemmas 2 and 3 directly prove this fact. Therefore, we need only consider the case $\lambda' = n+\kappa+1$ and $\lambda = n$. In this case, $q_{\lambda+1}...q_{\lambda'} = q_{n+1}...q_{n+\kappa+1} = r_{n+1}...r_{n+\kappa}q_{n+\kappa+1} = 10^{\kappa-1}q_{n+\kappa+1}$. To determine $q_{n+\kappa+1}$, we note that Q in Step (a) of the Pair Test has at most $\kappa-1$ successive 0's (note that Q begins with 1), and hence $\bar{Q}$ also has at most $\kappa-1$ successive 0's. Since $q_{n+\kappa+1}$ is preceded by $0^{\kappa-1}$, $q_{n+\kappa+1}$ must equal 1. Therefore, $\Delta\alpha = 2$ and by Lemma 2, $[s_\kappa 1]$ yields the same $(-o)$-string within both $\Upsilon(S)$ and $\Upsilon(R_\kappa)$. $\mathcal{QED}$ (Lemma 1).

Having addressed the start of R_k by Lemma 1, we now address the end of R_k. In particular, we examine how the symbols $r_{n-1}...r_{n+k+1}$ of R_k translate. Since $r_{n-1}...r_{n+k+1} = s_{n-1}r_n10^{k-1}u$, the final k symbols translate to $-^{k-1}o$ (Rules 2 and 3). Next, since s_{n-1} and r_n equal either 0 or 1, the substring $s_{n-1}r_n1$ exhibits four possibilities: 001, 011, 101, 111.

1. $s_{n-1}r_n = 00$ yields

$$\begin{aligned} s_{n-1}r_n10^{k-1}u &= 0[01]0^{k-1}u \\ &\to -[\sigma\tau] -^{k-1} o, \text{ for all } k \geq 1, \end{aligned} \tag{C.1}$$

   where Rule 2 yields the initial $-$ and the Pair Test yields $\sigma\tau$. The application of the Pair Test follows similar logic to Lemma 1. Skipping the details,

$$s_{n-1}r_n10^{k-1}u \to -o -^k o, \text{ for all } k \geq k_0, \tag{C.2}$$

where k_0 is the index of R_k at which $\sigma\tau$ first equals $o-$. It satisfies $k_0 \leq \kappa = n$.

2. $s_{n-1}r_n = 01$ yields

$$s_{n-1}r_n 10^{k-1}u = [01]10^{k-1}u \\ \to [-o] -^k o, \text{ for all } k \geq 1, \tag{C.3}$$

where the first two symbols are translated by a simple application of the Pair Test (omitted here) and the third, being an unpaired 1, by Rule 4.

3. $s_{n-1}r_n = 10$ yields

$$s_{n-1}r_n 10^{k-1}u = 1[01]0^{k-1}u \\ \to \sigma[\tau\omega] -^{k-1} o, \text{ for all } k \geq 1. \tag{C.4}$$

The Pair Rule yields $\tau\omega = -o$ for $k = 1$ and $\tau\omega = o-$ for $k > 1$. Hence,

$$s_{n-1}r_n 10^{k-1}u \to \sigma o -^k o, \text{ for all } k > 1, \tag{C.5}$$

where σ equals either $-$ or o.

4. For $s_{n-1}r_n = 11$, if $s_{n-1} = 1$ is paired with r_n,

$$s_{n-1}r_n 10^{k-1}u = [11]10^{k-1}u \\ \to [-o] -^k o, \text{ for all } k \geq 1, \tag{C.6}$$

where the first pair is translated by the Pair Test, using the fact that s_{n-2} must equal 1, and the third symbol by Rule 4.

If $s_{n-1} = 1$ is paired with s_{n-2}, then

$$...s_{n-1}r_n 10^{k-1}u = ...1][11]0^{k-1}u \\ \to ...\sigma]o -^k o, \text{ for all } k \geq 1, \tag{C.7}$$

where σ equals either $-$ or o and the pair [11] is translated by a simple application of the Pair Test.

Equations (C.3) and (C.6) imply that Cases 2 and 3, mentioned before Lemma 1, do not occur for any k. Thus, Lemma 1 proves Theorem 1 for $m < n$. Furthermore, Eqs. (C.2), (C.3), and (C.5)–(C.7) imply that $\Upsilon(R_k)$ ends in $o -^k o$ for all $k \geq k_0(n)$, where $k_0(n)$ is the first index at which this occurs and where $k_0(n) \leq n$. $\mathcal{QED}$ (Theorem 1).

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[6] For a more realistic distance to the detector, see Appendix B of Ref. [2].

[7] Due to the Coulomb singularity, the magnitude of the initial momentum is infinite, but its direction is nevertheless well defined, as seen in Fig. 4.

[8] The term "icicle" is borrowed from: L. Gottdiener, Mol. Phys. **29**, 1585 (1975); A. Tiyapan and C. Jaffé, J. Chem. Phys. **99**, 2765 (1993); **101**, 10393 (1994); **103**, 5499 (1995).

[9] K. A. Mitchell, J. P. Handley, B. Tighe, S. K. Knudson, and J. B. Delos, Chaos **13**, 880 (2003).

[10] In poetry, an "epistrophe" is a regular, repeated ending following possibly variable beginnings. It is appropriate here because we can predict how the epistrophe sequences end (they all have the same asymptotic structure), although we cannot always predict how such sequences begin nor can we predict every escape segment in the escape time plot (except by detailed numerical computation).

[11] In such a case, it is not obvious whether we should pick one of these three segments and regard it as a member of the minimal set, or whether the group of three segments should be regarded as a splitting of a single segment from the minimal set. This latter perspective is supported by the fact that all three segments have the same $(-o)$-string, as seen in Fig. 4.

[12] In poetry, a "strophe" is a stanza that may have irregular lines, so that it may break the regular structure of the poem.

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[14] For convenience, we allow ρ to take both positive and negative values. A "half-cycle" of ρ thus goes from zero to a maximum amplitude and back to zero again.

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[16] We justify this assertion by working with the parabolic coordinates (u, v) that are commonly introduced for the hydrogen problem, and we refer freely to the definitions and discussion of Sects. IIIA and IIIC of Ref. [2]. Consider first a point in the vp_v-plane (the surface of section defined by $u = 0$) that maps across the vertical axis $v = 0$, say from $v > 0$ to $v < 0$. In the uv configuration space this corresponds to a trajectory that passes from the positive v-axis around the origin to the negative v-axis. But such a trajectory, translated to the ρz coordinates, encircles the nucleus. Thus, mapping across the axis $v = 0$ in the vp_v-plane corresponds to encircling the nucleus. However, the line $v = 0$ in the vp_v-plane corresponds to $\mathcal{L}_0$ in the qp-plane. Thus, mapping across $\mathcal{L}_0$ in the qp-plane corresponds to encircling the nucleus.