Direct-interaction electrodynamics of a two-electron atom

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We study numerically the dynamical system of a two-electron atom with the Darwin interaction as a model to investigate scale-dependent effects of the relativistic action-at-a-distance electrodynamics. This dynamical system consists of a small perturbation of the Coulomb dynamics for energies in the atomic range. The key properties of the Coulomb dynamics are: (i) a peculiar mixed-type phase space with sparse families of stable non-ionizing orbits and (ii) scale-invariance symmetry, with all orbits defined by an arbitrary scale parameter. The combination of this peculiar chaotic dynamics ((i) and (ii)), with the scale-dependent relativistic corrections (Darwin interaction) generates the phenomenon of scale-dependent stability: We find numerical evidence that stable non-ionizing orbits can exist only for a discrete set of resonant energies. The Fourier transform of these non-ionizing orbits is a set of sharp frequencies. The energies and sharp frequencies of the non-ionizing orbits we study are in the quantum atomic range.

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The Coulomb dynamical system of the helium atom is a very peculiar chaotic system that exhibits Arnold diffusion [1], and with a typical trajectory having an infinity of possible time-asymptotic final states. For example, almost all negative-energy trajectories of Coulombian helium display the generic phenomenon of ionization, namely, the ejection of one electron [2]. Several nonlinear dynamical systems share this property of having more than one time-asymptotic final state, with the respective basins for each outcome having a complicated structure in initial condition space [3,4]. The numerical work on this paper is based on stable Coulombian orbits of a two-electron atom that do not ionize for several millions of turns of one electron around the nucleus. It is a property of the Coulomb dynamics of a two-electron atom that most initial conditions with a negative energy ionize very quickly in about 20 turns [2]. Then there are the very special initial conditions that do not ionize due to a precise phase balance between the two electrons. These rare non-ionizing orbits are defined very sharply in phase space and were first studied in reference [2] for plane orbits. Here we also develop a numerical procedure to search for non-ionizing orbits among a large number of possible tridimensional initial conditions.

The Coulomb Hamiltonian exhibits the scale invariance degeneracy: if we scale time and space as $t \rightarrow T t$, $\vec{r} \rightarrow L \vec{r}$, for $T^2/L^3 = 1$, the equations of motion are left invariant. For this reason, the behavior of the Coulomb dynamics is the same in all scales, a degeneracy which is broken by the relativistic effects of electrodynamics. The phenomenon of breaking the scale invariance in electrodynamics was explored analytically in [5] for the Darwin interaction, which is the low-velocity approximation to the Wheeler-Feynman action-at-a-distance electrodynamics. It was found in [5] that a simple resonant normal form approximation theory predicts a discrete set of quantized scales very close to the quantum atomic energies. Using these preliminary findings as guide, we present a numerical investigation of the stability of non-ionizing orbits for the Darwin dynamics and its dependence on the energy scale. It turns out that for energies of atomic interest, the Darwin equations of motion approximate the Coulomb equations plus a perturbation of size $\beta^2$, with $\beta \sim 10^{-2}$. Therefore, non-ionizing stable orbits of the Darwin dynamics should exist in the neighborhood of non-ionizing stable Coulombian orbits if the perturbation does not force ionization. For these, our numerical results with the Darwin dynamics indicate that the non-ionizing property plus stability require sharply defined discrete energies.

The Darwin interaction is not exactly a Lorentz invariant interaction [6,7], so we study it as an approximation to the relativistic action-at-a-distance electrodynamics, for the sake of including the present approach into an underlying physical theory. Maxwell’s theory would seem to be the natural candidate for the comprehensive physical theory, but it lacks time-reversibility and dipolar dissipation would forbid the orbits studied in this paper. There is also the choice of other more recent Lorentz-invariant Lagrangian systems and constrained Hamiltonian dynamical systems [8,9], whose exact forms are actually more amenable to numerical treatment than the Wheeler-Feynman electrodynamics, but we shall not consider them here. The interested reader should consult reference [2], where a covariant approximation to Wheeler-Feynman electrodynamics is attempted by the two-body Todorov equation of constraint dynamics.

This paper is organized as follows: in section I we review the state of the art of the time-reversible action-at-a-distance electrodynamics, and if the reader wants to skip this part the rest of the paper makes full sense as a
nonlinear dynamics study, except for the discussion at the end. In section II we describe the numerical calculations with the Coulomb limit of the Darwin interaction, find some non-ionizing orbits and their Fourier transforms. In section III we include the scale dependent Darwin terms and investigate the possibility of stable non-ionizing orbits. In section IV we put the conclusions and discussion.

I. ACTION-AT-A-DISTANCE ELECTRODYNAMICS

The Wheeler-Feynman [15] electrodynamics developed from the Schwarzschild-Tetrode-Fokker [16] direct-interaction functional. Equations of motion are derived from Hamilton’s principle for the action integral

\[ S = -\sum_i \int m_i c ds_i + e^2 \sum_{ij} \int \delta \left( \| x_i - x_j \|^2 \right) x_i \cdot x_j ds_i ds_j, \]

where the four-vector \( x_i(s_i) \) represents the four-position of particle \( i \) parametrized by arc-length \( s_i \), double bars indicate quadri-vector modulus \( \| x_i - x_j \|^2 = (x_i - x_j) \cdot (x_i - x_j) \) and the dot indicates the usual Minkowski relativistic scalar product of four-vectors. (Integration is to be carried over the hole particle trajectories, at least formally.) The above action integral describes an interaction at the advanced and retarded light-cones with an electromagnetic potential given by half the sum of action at the advanced and retarded light-cones with the Coulomb limit of the Darwin interaction, find nonlinear dynamics study, except for the discussion at the end. As far as understanding of the dynamics governed by the equations of motion, the state of the art is as follows: The exact circular orbit solution to the attractive two-body problem was proposed in 1946 [22] and rediscovered by Schild in 1962 [23]. The 1-dimensional symmetric two-electron scattering is a special case where the equations of motion simplify a lot and it has been studied by many authors, both analytically and numerically [24–26].

The Noether’s four-constant of motion derived from the Fokker Lagrangian involves an integral over the past history \[ P^\lambda = m_p \dot{x}_e^\lambda + e A^\lambda(x_p) + m_e \dot{x}_e^\lambda - e A^\lambda(x_e) \]

\[ -2 e^2 \int_\tau^\infty d\tau_p \int_{-\infty}^\tau d\tau_e \delta \left( \| x_e - x_p \|^2 \right) (x_p - x_e) \dot{x}_e \dot{x}_p, \]

\[ + 2 e^2 \int_\tau^\infty d\tau_p \int_{-\infty}^\tau d\tau_e \delta \left( \| x_e \|^2 \right) (x_p - x_e) \dot{x}_e \dot{x}_p, \]

where \( \delta \) represents the derivative of the delta function. Notice that because of this delta function, only finite portions of the trajectory are involved: actually an extent of length \( t \approx 2 r_{12}/c \) approximately. This non-local constant will behave very differently from the local Coulombian energy, that is known to confine orbits of a negative energy within a maximum separation distance. In the case where the particles acquire a large separation (unbound state), the hole past history is involved \( (t \approx 2 r_{12}/c \approx \infty) \) in the determination of the non-local energy constant.

As regards the mathematical structure of the equations of motion, for the case of a two-electron atom the acceleration of electron 1 is given by [27]

\[ a_1(t) = \frac{-e}{m \gamma^2} \left\{ E - \frac{v_1(t)}{c^2} E \cdot v_1(t) + \frac{v_1(t)}{c} \times B \right\}, \]

where \( -e \) and \( m \) are the electronic charge and mass, \( \gamma \equiv 1/\sqrt{(1 - v_1(t)/c)^2} \) and \( E \) and \( B \) are the total electric and magnetic fields produced by electron 2 and the nucleus.
In the action-at-a-distance theory these fields are given by the average of the retarded and advanced Lienard-Wiechert fields, calculated with the instantaneous position of the stationary nucleus and the retarded and advanced positions of electron 2 at the times \( t_2 = t_{\mp} \), which is defined by the implicit condition

\[
R_{\mp} \equiv |r_2(t_{\mp}) - r_1(t_1)| = \mp ct_{\mp} - t_1,
\]

where the minus and plus signs are the conditions for the retarded and advanced times respectively. The partial electric fields of electron 2 acting on electron 1 at time \( t_1 \) are \([28]\)

\[
E_-(x_1, x_2-, v_2-, a_2-) = \frac{-e(n_- - \beta_2)}{\gamma_2^2(1 - n_- \cdot \beta_2)^3R_-^2}
\]

\[
- \frac{e}{c} \left[ \frac{n_- \times \{(n_- - \beta_2) \times \beta_2\}}{(1 - n_- \cdot \beta_2)^3R_-} \right],
\]

where \( R_{\mp}n_{\mp} \equiv r_2(t_{\mp}) - r_1(t_1) \), \( \beta_2 \equiv v_2/c, (e^-), \gamma_2 \equiv (1 - \beta_2^2)^{-1/2} \) and \( c \) is the speed of light. The advanced field \( E_+ \) is obtained from the above expression by replacing \( t_- \) by \( t_+ \) and \( c \) by \( -c \). The partial magnetic fields of electron 2 are

\[
B_{\mp} = \pm n_{\mp} \times E_{\mp},
\]

where the \( \pm \) is to ensure an outgoing Poynting vector \((cE \times B)\) for the retarded fields and an incoming Poynting vector for the advanced fields. The total electric field in equation (1) must include also the instantaneous Coulomb electric field of the stationary nucleus.

Equation (1) can suggest a paradox about causality, as the force depends on the future of particle 2. In the following, and to finish this introduction, we show that equation (1), when written properly, becomes a functional differential equation with delayed argument only, as first observed in [24]. To outline the essentials of the explanation, let us first ignore the field of the nucleus and take the nonrelativistic limit of (1) \((v_1 = 0)\). In this approximation the electric field \( E \) entering in equation (1) evaluates to

\[
E = 0.5E_+(x_1, x_2+, v_2+, a_2+) + 0.5E_-(x_1, x_2-, v_2-, a_2-).
\]

Then we note that one can use equation (1) as an equation of motion for particle 2, by solving the rearranged form of (1),

\[
eE_+(x_1, x_2+, v_2+, a_2+) = -2ma_1(t) - eE_-(x_1, x_2-, v_2-, a_2-),
\]

for the most advanced acceleration of particle 2, \( a_{2+} \equiv a_2(t + \frac{dt_+}{c}) \). In the above form it is clear that the right hand side involves only functions evaluated at times prior to the most advanced time, defined by \( s = t + \frac{dt_+}{c} \), and no further advanced information is necessary, eliminating the ghost of dependence on the future. In the same way, the causal equation of motion of particle 1 is to be produced from the equation for particle 2 by solving for the most advanced acceleration of particle 1. For the special case of 1-dimensional motion of two electrons, \( E_+ = E_+(x_1, x_2+, v_2+) \) depends only on the advanced velocity, and (1) can easily be solved for this advanced velocity as a function of the past history. In the 3-dimensional case there is an extra complexity, as the acceleration appears in the Lienard-Wiechert partial field \( E_+ \) in the form \( n_{12} \times (n_{12} \times a_{2+})/r_{12} \). The bad news is that the component of the acceleration along the advanced normal can not be solved for from the value of the double-vector-product only. Because of this degeneracy, equation (1) is an algebraic-differential equation, and the null direction of the left hand side of (1) is a constraint to be satisfied by the right hand side (the scalar product with \( n_{12} \) must vanish). The numerically correct way to integrate this type of equation is by use of the modern integrators for algebraic-differential equations like DASSL adapted for retarded equations (which has never been done yet) or by dealing directly with the algebraic constraint [31]. According to the standard classification of G. A. Kamenskii [32], equation (1) belongs to the class of differential-difference equations of neutral type. Even though more complex, the motion is still causally determined by the past trajectory, as we wanted to demonstrate, the price being an algebraic neutral delay equation.

As far as initial conditions go, the general theory on delay equations [32] tells us that we need to provide an initial \( C^2 \) function describing the position of particle 2 from \( s - \frac{dx_2}{c} = t - \frac{dt_+}{c} \) up to the initial instant \( s = 0 \). The information on particle 1 needed is also to be provided over twice the retardation lag seen by particle 1. This is a short piece of trajectory for bound nonrelativistic atomic orbits, but for a ionized state or a runaway orbit this can be the whole past history! Unless further simplifications or conditions are added, this is the generic problem at hand. The 3-dimensional cases of atomic interest (e.g. helium) have never been studied, and they are more complex than the 1-d scattering problem. The only existing analytical result in the 3-dimensional case is the linear stability of the Schonberg-Schild circular orbits [27], resulting in an infinite number of unstable solutions to the characteristic equation. The numerical treatment of these equations displays instabilities and is generally difficult. In the following we resort to the Darwin approximation not as much as a mathematical approximation to the action-at-a-distance electrodynamics, but
as a physical approximation of Lorentz-invariant dynamics in the atomic (shallow) energy range.

II. NUMERICAL CALCULATIONS FOR THE COULOMB DYNAMICS

To introduce our numerical calculations, we start from the scale-invariant Coulomb limit of the Tetrode-Fokker-Wheeler-Feynman interaction: Let $-e$ and $m$ be the electronic charge and mass respectively and $Ze$ the nuclear charge of our two-electron atom, which in this work is assumed to have an infinite mass. All our numerical work uses a scaling which exploits the scale invariance of the Coulomb dynamics: Given a negative energy, there is a unique circular orbit at that energy with frequency $\omega_o$ and radius $R$ related by $e^2/(m\omega_o^2R^3) = 1/(Z - \frac{1}{2}) \equiv \zeta(Z)$. We scale distance, momentum, time and energy as $x \to Rr$, $p \to m\omega_oRp$, $\omega_odt \to dr$ and $E \to m\omega_o^2R^2\hat{H}$, respectively. In these scaled units, the Coulomb dynamics in the atomic (shallow) energy range is described by the scaled Hamiltonian

$$\hat{H} = \frac{1}{2}(\hat{p}_1^2 + \hat{p}_2^2) + \zeta(Z)(\frac{1}{r_{12}} - \frac{Z}{r_1} - \frac{Z}{r_2}),$$

where $r_1 \equiv |\vec{x}_1|$, $r_2 \equiv |\vec{x}_2|$, $r_{12} \equiv |\vec{x}_1 - \vec{x}_2|$ (single bars represent euclidean modulus) and $\beta \equiv \omega_oR/c$. For a generic non-circular orbit, $\beta$ plays the role of a scale parameter, and we recover the value of the energy in ergs through $E = mc^2\beta^2\hat{H}$. Notice that $\beta$ does not appear in the scaled Hamiltonian, which is the scale invariance property. From the scaled frequency $\hat{w}$ and scaled angular momentum $\hat{l}$ we can recover the actual values in CGS units by the formulas

$$w = \frac{mc^2\zeta(Z)\hat{p}^3}{e^2/c} \hat{w}, \quad l = \frac{e^2/c}{\zeta(Z)} \hat{l}.$$

The only other analytic constant of the Coulomb dynamics, besides the energy $\zeta(Z)$, is the total angular momentum, and this dynamics in chaotic and displays Arnold diffusion, as proved in [3] for a similar three-body system.

The numerical calculations were performed using a 9th-order Runge-Kutta embedded integrator pair [3]. We chose the embedded error per step to be $10^{-14}$, and after ten million time units of integration the percentage changes in energy and total angular momentum were less than $10^{-6}$. As a numerical precaution we performed the numerical calculations using the double Kustanheimo coordinate transformation to regularize single collisions with the nucleus [3]. As these alone are not enough for faithful integration, we checked that there was never a triple collision, as the minimum inter-electronic distance was about 0.3 units while the minimum distance to the nucleus was 0.01 units for all the orbits considered in this work. We also checked that along stable non-ionizing orbits we can integrate forward up to fifty thousand time units, reverse the integration, go backwards another fifty thousand units and recover the initial condition with a percentile error of $10^{-5}$. For longer times this precision of back and forth integration degenerates rapidly, which is due to the combined effect of numerical truncation and stochasticity. The question of how far in time the numerical trajectories approximate shadowing trajectories in the present system is far from trivial [37], but we assume it to be a time at least of the order of these one hundred thousand units. (Energy conservation of one part in a million is achieved for much longer times, even one billion time units).

The study of orbits of a two-electron atom was greatly stimulated by the recent interest in semiclassical quantization, and these studies discovered two types of stable zero-angular-momentum periodic orbits for helium ($Z = 2$): the Langmuir orbit and the frozen-planet orbit [36,37]. A detailed study of the non-ionizing orbits of Coulombian helium was initiated in reference [3] for plane orbits, and we describe some of their results below. There are basically two types of non-ionizing orbits:

Symmetric if $r_1 = r_2$ for all times and asymmetric if $r_1 \neq r_2$ generically. Symmetric orbits are produced by symmetric initial conditions like for example $x_1(0) = -x_2(0)$ and $v_1(0) = -v_2(0)$ or $x_1(0) = -x_2(0)$ and $v_1(0) = v_2(0)$ with $x_1(0) \cdot v_1(0) = 0$ [38]. Because $\zeta(Z)$ is symmetric under particle exchange, these orbits satisfy $r_1 = r_2$ at all times, and therefore cannot ionize if $H < 0$ (both electrons would have to ionize at the same time, which is impossible at negative energies). For example the double-elliptical orbits (two equal ellipses symmetrically displaced along the x-axis) discussed in [3] are in this class. Double-elliptical orbits are known to be unstable [39] and we find that they ionize in about one hundred turns because of the numerical truncation error. Most symmetric plane orbits are very unstable to asymmetric perturbations, with the exception of the Langmuir orbit for a small range of $Z$ values around $Z = 2$. [39]

The simplest way to produce an asymmetric non-ionizing plane orbit is from the initial condition $x_1 = (r_1, 0, 0)$, $\dot{x}_1 = (0, v_1 \sqrt{4/7}, 0)$, $x_2 = (-1, 0, 0)$, $\dot{x}_2 = (0, -\sqrt{4/7}, 0)$, as suggested in [38]. In Figure 1 we show the electronic trajectories for the first three hundred scaled time units along a two-dimensional non-ionizing orbit of $Ca^{+18}(Z = 20)$ with $r_1 = 1.4$ and $v_1 = 1.28442$ in the above defined condition. We used a numerical refining procedure to finely adjust $v_1$ as to maximize the non-ionizing time and this condition of Figure 1 does not ionize for one million time units. The orbit survives that far only for a very sharp band of values of $v_1$, other neighboring values producing quick ionization. This orbit was named double-ring torus in [3]. The other possible type of non-ionizing orbit resulting from the above initial condition, depending on $(r_1, v_1)$, is what was named braiding torus in reference [3], with both electrons orbiting within
the same region. A search over \((r_1, v_1)\) was conducted in [2], and it was found that most values of \((r_1, v_1)\) produce quick ionization except for a zero-measure set of \((r_1, v_1)\) values where braiding tori or double ring orbits are found. This suggests the general result that non-ionizing orbits are rare in phase space.

To search for general tridimensional non-ionizing orbits in phase space, it is convenient to introduce canonical coordinates \(\vec{x}_d\) and \(\vec{x}_c\)

\[
\begin{align*}
\vec{p}_d &\equiv (\vec{p}_1 - \vec{p}_2)/\sqrt{2}, & \vec{x}_d &\equiv (\vec{x}_1 - \vec{x}_2)/\sqrt{2}, \\
\vec{p}_c &\equiv (\vec{p}_1 + \vec{p}_2)/\sqrt{2}, & \vec{x}_c &\equiv (\vec{x}_1 + \vec{x}_2)/\sqrt{2}.
\end{align*}
\]  
\tag{5}

Initial conditions with \(\vec{x}_c = \vec{p}_c = 0\) describe double-elliptical orbits (and circular as a special case). To generate an elliptical initial condition, we exploit the scale invariance and set the energy to minus one. It is easy to check that elliptical orbits of the Hamiltonian (3) with an energy of minus one must have a total angular momentum of magnitude ranging from zero to two. To exploit the rotational invariance of (3), we can choose the plane defined at \(\vec{x}_c = \vec{p}_c = 0\) by the angular momentum \(\vec{L} = \vec{x}_d \times \vec{p}_d + \vec{x}_c \times \vec{p}_c = \vec{x}_d \times \vec{p}_c\) to be the \(xy\) plane. On this \(xy\) plane a single number \(0 < |\vec{x}_d \times \vec{p}_d| < 2\) (the angular momentum), determines completely the elliptical orbit. The next step in producing a generic orbit is to add all possible perturbations along \(\vec{x}_c\) and \(\vec{p}_c\) to the chosen elliptical orbit. These are six directions and once we are looking for bound oscillatory orbits, we can choose \(z_c = 0\), once \(z_c\) has to cross the \(xy\) plane at some point. These are five numbers to vary and plus the angular momentum of the elliptical orbit it totals six parameters. Our numerical search procedure consists in varying these six parameters over a fine grid, integrating every single initial condition until the distance from one electron to the nucleus is greater than twenty units, which is our ionization criterion. This criterion fails if the orbit has a very low angular momentum because these can go far away from the nucleus and come back, and therefore our search possibly misses low-angular-momentum non-ionizing orbits. As the majority of the initial conditions ionize very quickly, this search procedure is reasonably fast. We first perform a coarse search for ionization times above one thousand units and then refine in the neighborhood of each surviving condition to get conditions that do not ionize after one million time units.

Using the above numerical search procedure we found the tridimensional non-ionizing initial condition of Figure 2 for helium, a tridimensional double-ring orbit generated by the initial condition

\[
\begin{align*}
x_1 &= (1.2812617, 0.0147169, 0.0) \\
x_2 &= (-1.5511484, 0.0147169, 0.0) \\
p_1 &= (-0.0194868, 0.4398889, 0.1094930) \\
p_2 &= (-0.0194868, -0.7972467, 0.1094930),
\end{align*}
\]

which does not ionize before ten million turns. (After the search and refinement, we scaled this orbit’s energy to minus one, for later convenience). We also found the non-ionizing orbit orbit of Figure 3 for H-minus \((Z = 1)\), a tridimensional orbit generated by the condition

\[
\begin{align*}
x_1 &= (1.9776507, -0.3411364, 0.0) \\
x_2 &= (-1.2288121, -0.3411364, 0.0) \\
p_1 &= (0.0421302, 0.5057782, 0.2810539) \\
p_2 &= (0.0421302, -0.4132970, 0.2810539),
\end{align*}
\]

which does not ionize before one million turns (Coulombian energy of this condition is also minus one). This last orbit is fragile and numerically harder to find: as the first electron has an orbit very close to the positive \(Z = 1\) charge, there remains only a dipole field to bind the second electron. As the outer electron is much slower in the scaled units, we had to plot the first 10000 time units of evolution to display the generic features of the trajectory.

Non-ionizing orbits of \(H^-\) are very rare in phase space, which is reminiscent of the quantum counterpart, as the \(H^-\) ion is known to have only one quantum bound state at \(E \simeq -0.55mc^2\alpha^2\), very close to the ionization threshold \((-0.5mc^2\alpha^2)\).

One remarkable fact about these non-ionizing orbits is that they all have a very sharp Fourier transform. This property makes them approximately quasi-periodic orbits. For example in Figure 4 we plot the fast Fourier transform of the orbit of Figure 2, performed using \(2^{16}\) points. (It seems that there are at least two basic frequencies in the resonance structure of Figure 4). Even though these orbits look like quasi-periodic tori, there seems to be a thin stochastic tube surrounding each orbit, as evidenced by a small positive maximum Lyapunov exponent. We calculated numerically this maximum Lyapunov exponent by doubling the integration times up to \(T = 10^7\) and found that the exponent initially decreases but then saturates to a value of about 0.001 for the orbits of Figures 1, 2 and 3. The gravitational three-body problem has recently been proved to display Arnold diffusion [3], and this numerically calculated positive Lyapunov exponent suggests that the same is true for the two-electron Coulombian atom.

**III. NUMERICAL CALCULATIONS FOR THE DARWIN DYNAMICS**

The numerical integrations in this section are performed using the Darwin approximation. The Darwin equations of motion are a \(\beta^2\) perturbation of the Coulomb dynamics, of size \(\beta^2 \sim 10^{-4}\) for atomic energies. In the scaled units of section II the Darwin Hamiltonian is the following \(\beta^2\) perturbation of Hamiltonian (3)

\[
\hat{H}_D = \frac{1}{2}(|\vec{p}_1|^2 + |\vec{p}_2|^2) + \zeta(Z)\left\{ \frac{1}{r_{12}} - \frac{Z}{r_1} - \frac{Z}{r_2} \right\}
\]
\[-\frac{\zeta(Z)\beta^2}{2r_{12}^2} - (\hat{n}_{12} \cdot \hat{p}_1)(\hat{n}_{12} \cdot \hat{p}_2)] - \frac{\beta^2}{8}(||\hat{p}_1||^4 + ||\hat{p}_2||^4), \tag{6}\]

where \(\hat{n}_{12} \equiv (\vec{x}_1 - \vec{x}_2)/r_{12}\). The second line represents the Biot-Savart magnetic interaction plus the first relativistic correction to the static electric field and the last line describes the relativistic mass correction. Notice that these are both proportional to the small parameter \(\beta^2\), which makes them a small scale-dependent perturbation on the scale invariant Coulomb Hamiltonian (first line). It is possible to regularize the Darwin equations with the same double-Kustanheimo transformation \([34]\), only that here one needs to define the regularized time using the higher powers \(dt = r_1^2 r_2^2 ds\), instead of the lower powers \(dt = r_1 r_2 ds\) used to regularize the Coulomb equations \([34]\).

The main question we address numerically in this section is the dependence of the stability of a non-ionizing orbit with the energy scale of the orbit. Here we use the word stability to mean ionization-stability: We call an initial condition ionization-stable if any small perturbation of it produces another non-ionizing orbit. The scale-dependent Darwin terms (of size \(\beta^2\)) produce significant deviations from the Coulomb dynamics only in a time-scale of order \(1/\beta^2\), which we find numerically to be the typical time for a non-ionizing Coulombian initial condition to ionize along the Darwin vector field. This poses a numerical difficulty if \(\beta\) is too small because one has to integrate the orbit for very long times to investigate the stability. It turns out that ionization-stable orbits can be found at larger values of \(\beta\) for larger values of \(Z\). Here the dynamical stability mechanism is reminiscent of quantum atomic physics, where the values of \(\beta\) vary with the nuclear charge as \(\beta \sim Z/137\). Large values of \(Z\) facilitate the numerical procedure and in the following we present the numerical investigation of the stability of non-ionizing orbits starting from the large \(Z\) case.

Let us start with the \(Z = 20\) calcium ion two-electron system along the non-ionizing orbit of Figure 1 by fixing \(r_1 = 1.4\) and \(v_1 = 1.28442\), in the condition defined in section II. To test the stability of the orbit at each value of \(\beta\) we add a random perturbation of average size \(\beta^2\) to the initial condition and integrate the Darwin dynamics until either we find ionization or the time of integration is greater than \(10^7\) time units. We repeat this for at least twelve randomly chosen perturbations (because of the twelve degrees of freedom) and the minimum time to ionization is plotted in Figure 5 as a function of \(\beta\). It can be seen that only for a narrow set of values around \(\beta \sim 0.037\) this minimum time to ionization was greater than \(10^6\), or the other values it decreases rapidly to a value of about \(10^3\). One could argue that for the other values of \(\beta\) the non-ionizing initial condition has shifted away from the \(v_1 = 1.28442\) initial condition and this being the reason that our orbit ionized. To test this, we fixed \(\beta\) at a "bad" value for example \(\beta = 0.02\) and varied the plane initial condition in the neighborhood of this condition of Figure 1. We found that the minimum time to ionization was always about \(10^5\) (also the maximum time before ionization was about \(10^3\)). We also searched in a bigger neighborhood, of size proportional to \(\beta\). This suggests the interpretation that for the special resonant value of \(\beta = 0.037\) the net diffusive effect of the scale-dependent term vanishes, allowing a non-ionizing perturbed manifold. In order to have a direct interpretation (in atomic units) of the scale parameter \(\beta\), it is convenient to scale to minus one the energy of the initial condition of Figure 1 (by exploiting the Coulombian scale invariance). After this, the energy of the orbit in ergs evaluates to \(E = mc^2 \beta^2 \hat{H} = -mc^2 \beta^2\), and for \(\beta = 0.037\) this is approximately \(-24.59\) atomic units. The total angular momentum of this orbit is \(l_z = 7.94\alpha\). This orbit’s energy is above the ionization continuum of the ion, \(E = -mc^2 \alpha Z^2/2 = -200\) atomic units, but it is still in the quantum range. It serves nevertheless to demonstrate that this dynamical system might exhibit non-ionizing stable orbits only at very sharply defined energy values.

For the orbits of Figures 2 and 3, the above procedure becomes prohibitively slow, as the value of \(\beta\) are much smaller and one must integrate for very long times, much beyond the estimated shadowing time. To partially overcome this we used a larger amplitude random perturbation (of average size \(20\beta^2\)), to produce faster ionization. The drawback with this is that the minimum ionization time does not show pronounced peaks, only the average ionization time still showing a signature of scale dependence. In Figure 6 we show this average time for the orbit of Figure 3. This property of sharply defined energies can possibly be found for the lower-lying energies below the ionization threshold as well. These orbits would involve configurations where the electrons come very close to the nucleus and acquire a large velocity. Even though our integrator is regularized, the correct physical electronic repulsion is greatly amplified when one electron has a relativistic velocity and the Darwin approximation can not describe the physics then. Actually, it is known that the Darwin interaction can produce unphysical effects when pushed to relativistic energies \([1]\). We therefore do not expect to find these low-lying atomic energy scales with the present Darwin approximation and shall be content with these interesting result already.

For the same reason given above, we do not study here the frozen-planet periodic orbit (the two electrons performing one-dimensional periodic motion on the same side of the nucleus, with the inner electron rebounding from the origin, an artifact of regularization). The main problem being the failure of the Darwin approximation, as the inner particle goes to the speed of light \([12]\). The
correct relativistic dynamics can actually produce a new physical inner turning point very close to the origin but not at the origin as the regularized motion, and we discuss elsewhere [12].

Last, we consider the non-ionizing symmetric periodic orbit called the Langmuir orbit, where the two electrons perform symmetric bending motion shaped approximately like a semi-circle [37]. For the Coulomb two-electron atom with \( Z = 2 \) this orbit was found to have a zero maximum Lyapunov exponent [36]. The orbit is therefore neutrally stable, which is the best one can expect from a periodic orbit of a Hamiltonian vector field. (Absolute stability violates the symplectic symmetry, which says that to every stability exponent \( \lambda \) one should have a \( 1/\lambda \) exponent). It is a simple matter to obtain the Langmuir-like orbit for the Darwin Hamiltonian at any given value of \( \beta \) all it takes is a little adjusting in the neighborhood of the Coulombian Langmuir condition. We attempted to investigate numerically any scale-dependent diffusion away from this Darwin-Langmuir condition for \( \beta \) in the atomic range, but again the numerics is prohibitively slow at the time of writing this work.

IV. CONCLUSIONS AND DISCUSSION

The simplified dynamical mechanism behind resonant non-ionization seems to go intuitively as follows: The peculiar scale-invariant Coulomb dynamics determines the non-ionizing orbits within narrow "stochastic tubes". The next step is the action of the small scale-dependent relativistic corrections that produce a slow diffusion of the orbit out of the thin tube in a time of the order of \( 1/\beta^2 \). After this, quick ionization follows. Only at very special resonant values of \( \beta \) the relativistic terms leave the orbit within the tube, a resonant effect that depends on \( \beta \), fixing the energy scale. In the literature, the escape to infinity from simpler to understand two-degree-of-freedom systems has been attributed to cantori, which, as is well known, can trap chaotic orbits near regular regions for extremely long times [4]. In the present larger dimensional case it appears that resonances are also controlling the escape to infinity of one electron by the existence of extra resonant constants of motion [12]. This seems to be in agreement with the numerical results of very sharp peaks for the minimum ionization time. We have tried to concentrate on the physics described by this combination of chaotic dynamics on a two-electron atom with inclusion of relativistic correction, while discussing this highly nontrivial result of nonlinear dynamics.

In references [11] we noticed that a simple resonant normal form criterion gives a surprisingly good prediction for the discrete atomic energy levels of helium. The resonant structure was calculated using the Darwin interaction [3], which is the low-velocity approximation to both Maxwell’s [4] and Wheeler-Feynman’s [7] electrodynamics. As we saw in section II, the Coulombian non-ionizing orbits are far from circular, and these orbits would radiate even in dipole according to the time-reversible Maxwell’s electrodynamics (circular orbits radiate only in quadrupole but are linearly unstable). It becomes then clear that the heuristic results of [11] can only have a physical meaning in the context of a time-reversible theory (as the action-at-a-distance electrodynamics for example).

The combination of chaotic dynamics with relativistic invariance has never been explored numerically, and most known Lorentz-invariant dynamical systems are for one particle and possess trivially integrable dynamics. The situation gets unexpectedly much more complicated for more than one particle (apart from the trivial non-interacting many-particle system): Due to the famous no-interaction theorem [10], the relativistic description of two directly interacting particles is impossible within the Hamiltonian formalism and its set of ten canonical generators for the Poincare group [14]. Description of interacting particles is possible only in the context of constraint dynamics, with eleven canonical generators and with the Dirac bracket replacing the Poisson bracket. For example the relativistic action-at-a-distance equations for two interacting electrons are non-local and possess only infinite-dimensional constrained Hamiltonian representations [24, 12]. The interested reader should consult some recently found two-body direct-interaction relativistic Lagrangian dynamical systems [11] as well as the constraint-dynamics direct-interaction models recently used in chromodynamics and two-body Dirac equations [26, 44]. The nonlinear dynamics of these models could display interesting and so far unexplored dynamical behaviour.

It would be natural to wonder if one can find an analogous scale-dependent dynamics for a dynamical system describing the hydrogen atom, apparently the simplest example of Lorentz-invariant two-body relativistic dynamics of atomic interest. It turns out that hydrogen is not simpler than helium at all, but it appears to us that there is an essential difference which has actually made the interesting dynamics of a two-electron atom amenable to study already within the Darwin approximation: In a two-electron atom orbits with a negative energy can ionize, while in hydrogen this might be possible only if one includes all orders of the relativistic action-at-a-distance interaction. (As we saw in section I, the "Noether’s energy constant" involves a segment of the past trajectory, and a negative value does not forbid ionization.) Ionization with a negative energy would be impossible for hydrogen within the Darwin approximation (unless the electron goes to the speed of light). This is indication that in hydrogen the essential physics described by the action-at-a-distance electrodynamics is of non-perturbative character. The paradoxical result of
the infinite linear instability of circular orbits in atomic hydrogen \cite{27} is another warning of this non-perturbative dynamics.

V. ACKNOWLEDGMENTS

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FIG. 1. Non-ionizing double-ring orbit for Ca$^{+18}$ ion ($Z = 20$), obtained from the initial condition $x_1 = (r_1, 0, 0)$, \( \dot{x}_1 = (0, v_1 \sqrt{4/7}, 0) \), $x_2 = (-1.0, 0, 0)$, \( \dot{x}_2 = (0, -\sqrt{4/7}, 0) \), with $r_1 = 1.4$ and $v_1 = 1.28442$, trajectories are shown for the first 300 time units, the inner ring represents the orbit of electron 1 and the outer ring represents the orbit of electron 2, the units are the scaled units defined in section II.

FIG. 2. Non-ionizing double-ring tridimensional orbit for helium ($Z = 2$), trajectories are shown for the first 200 time units, the inner ring represents the plane projection of the orbit of electron 1 and the outer ring represents the projection of the orbit of electron 2. Positions are in the scaled units defined in section II.

FIG. 3. Non-ionizing tridimensional orbit for H-minus ($Z = 1$), trajectories are shown for the first 10000 time units. The inner ring represents the plane projection of the orbit of electron 1 and the outer ring represents the projection of the orbit of electron 2. Trajectory of the (fastest) electron 1 winds almost everywhere in the the dark inner core of figure. Positions are measured in the scaled units of section II.

FIG. 4. Fast Fourier Transform of the orbit of Figure 2 using $2^{16}$ points. Frequencies are measured in the scaled units of section II.

FIG. 5. Minimum time to ionization (among 24 random perturbations of average size $\beta^2$ added to the orbit of Figure 1) $\beta$ is the adimensional parameter and time is measured in the scaled units of section II.

FIG. 6. Average time to ionization (among 12 random perturbations of average size $20\beta^2$ added to the orbit of Figure 3) $\beta$ is the adimensional scale parameter and time is measured in the scaled units of section II.
