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On the one-dimensional helium atom

A López-Castillo, M A M de Aguiar and A M Ozorio de Almeida

Instituto de Fíisica 'Gleb Wataghin', Universidade Estadual de Campinas, CP 6165, Campinas, SP, 13081-970, Brazil

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Abstract. A careful discussion of the interaction of the inner electron with the nucleus of the helium atom allows for the reduction to a one-dimensional Hamiltonian describing the *frozen planetary atom* configuration. This is obtained by cancelling the angular momentum of each electron, even though it is only their sum which is guaranteed to be constant. The true oscillatory nature of the angular momenta in the full two-dimensional Hamiltonian can be included in a time-periodic model that correctly accounts for the finite lifetime of the frozen planetary atom. This system can be further simplified by averaging over the motion of the inner electron so as to define an oscillatory Hamiltonian with a single degree of freedom.

1. Introduction

There has been increasing interest in new configurations for classical motion of the helium atom. It is known that chaotic and regular motion coexist in this quintessential three-body problem. Detailed knowledge of this system is necessary for the understanding of the semiclassical limit of the quantum helium atom. In spite of the inherent difficulties the balance of electronic charges obviously favours collinear configurations for the nucleus and the two electrons. This opens the possibility of approximate models in one spatial dimension. The purpose of this paper is to discuss the general derivation of such existing models and the way that they can be refined.

Taking $\boldsymbol{r}_i$ as the position vector of the ith electron in Cartesian coordinates and $\boldsymbol{p}_i$ as the corresponding momentum, we obtain the Hamiltonian

$$H = \frac{1}{2}(p_1^2 + p_2^2) - \frac{2}{|\boldsymbol{r}_1|} - \frac{2}{|\boldsymbol{r}_2|} + \frac{1}{|\boldsymbol{r}_1 - \boldsymbol{r}_2|} \tag{1}$$

in the approximation where the nucleus has infinite mass. This system with six freedoms, would decouple into two three-freedom hydrogenic atoms in the absence of the last term in (1). So it shares with the hydrogen atom the problems of a singular Hamiltonian, to which it adds non-integrability due to the non-perturbative interelectronic repulsion.

The most delicate task is to find realistic ways in which to reduce the dimension of the phase space. Conservation of energy and total angular momentum bring this down from 12D (twelve dimensions, fixing the nucleus at the origin) to 8D. If the initial positions and velocities are in the same plane, it will remain invariant. In this special case of a spatially 2D system we have an 8D system in phase space that is reduced to 6D by conservation of energy and total angular momentum. There is no general *a priori* justification for the further drastic reduction to one spatial dimension with which we are concerned here, i.e. of a 4D system restricted to 3D by energy conservation. However, the simplification is so great

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that it is worth pursuing as a pointer to regimes of motion that can then be investigated in higher dimensions. Indeed, an approximate spatial 1D regime known as the *frozen planetary atom* (FPA) has been observed experimentally [1] and numerically [2]. This motion is characterized by the outer electron remaining at an approximately fixed distance from the nucleus while the inner electron oscillates.

Here we do not have the ambition of explaining why the FPA is stable as opposed to other possible configurations. Our purpose is to establish, given that this approximately linear motion was found numerically, what is the most realistic effective 1D Hamiltonian to use.

2. Theory and numerical results

In the 1D version of (1) there is nothing that prevents the inner electron from colliding with the Coulomb singularity at the origin. Traditionally the hydrogenic singularities can be dealt with by regularizing the Hamiltonian [3] or by smoothing. Regularization was originally developed for planetary motion [4]. The idea is to divide the Hamiltonian by the divergent function and then to make an appropriate canonical transformation. Smoothing merely substitutes $|\boldsymbol{r}_i|$ by $(r_i^2+\delta^2)^{1/2}$ in the second and third terms in (1). We need not worry about the singularity in the last term, since orbits of finite energy cannot access it, except for the triple collision [4].

Let us consider the helium Hamiltonian (1) in polar coordinates $|\boldsymbol{r}_i|, \theta_i$, with conjugate momenta $\boldsymbol{\Pi}_i, \boldsymbol{l}_i$

$$H=\frac{1}{2}(\Pi_1^2+\Pi_2^2)-\frac{2}{|\boldsymbol{r}_1|}-\frac{2}{|\boldsymbol{r}_2|}+\frac{l_1^2}{2r_1^2}+\frac{l_2^2}{2r_2^2}+\frac{1}{|\boldsymbol{r}_1-\boldsymbol{r}_2|}\,. \tag{2}$$

Approximate 1D motion will occur if both the angular momenta remain small throughout the motion. However, this will allow very close collisions of the inner electron r_1 with the nucleus at the origin, because of the small strength of the centrifugal barrier ${l_1}^2/2{r_1}^2$. During the short time in which the collision takes place, we may neglect the interelectronic interaction. The orbit of the inner electron will then be the segment of a very eccentric ellipse as shown in figure 1.

Projecting the 2D motion onto the Ze_2 line in figure 1, we see that there will inevitably be a transition from the Zee configuration to eZe and back again. Though this is allowed for in the 1D version of (1) if the singularity at the origin is smoothed, this procedure would not force the configuration back to Zee. Conversely, regularization at the origin can only be achieved separately for the Zee and the eZe configurations as sketched in figure 2.

2.1. One-dimensional models

The best way to justify the 1D model depends on the fact that close to the Zee configuration

$$|\boldsymbol{r}_1-\boldsymbol{r}_2|\simeq||\boldsymbol{r}_2|-|\boldsymbol{r}_1|| \tag{3}$$

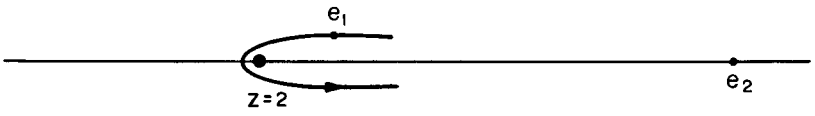

Figure 1. Inner electron going around the nucleus in an almost elliptic and very eccentric orbit: during a short time interval the Zee configuration changes to eZe.

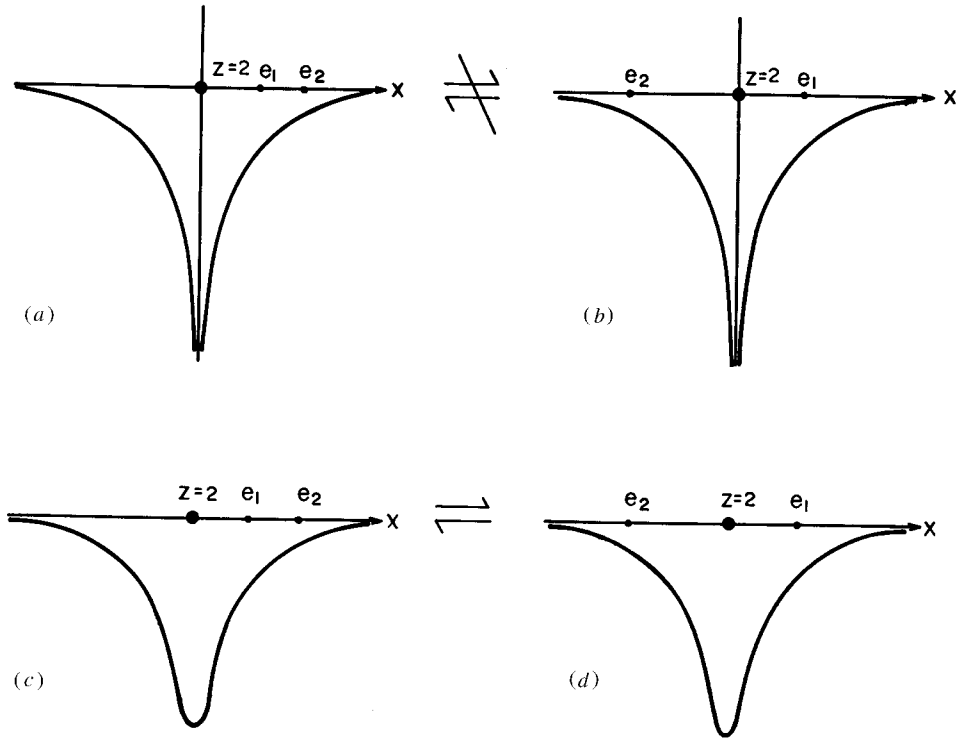

Figure 2. Schematic representation of the *Zee* and *eZe* configurations for the regularized model (*a*) and (*b*), and smoothed model (*c*) and (*d*).

whereas for the eZe we may approximate

$$|\boldsymbol{r}_1 - \boldsymbol{r}_2| \simeq |\boldsymbol{r}_2| + |\boldsymbol{r}_1| \,. \tag{4}$$

If the nearly collinear motion starts as *Zee*, there will only be a very short time for which (3) is not valid. Moreover, this only happens at the collision, when the inter-electronic term is relatively small. Furthermore, the difference between (3) and (4) can be neglected when $|r_1| \ll |r_2|$, so by all accounts we can approximate (2) by

$$H_{Zee} = \frac{1}{2}(\Pi_1^2 + \Pi_2^2) - \frac{2}{|\boldsymbol{r}_1|} - \frac{2}{|\boldsymbol{r}_2|} + \frac{l_1^2}{2r_1^2} + \frac{l_2^2}{2r_2^2} + \frac{1}{||\boldsymbol{r}_2| - |\boldsymbol{r}_1||} \tag{5}$$

when both the angular momenta are small and the motion starts in the Zee configuration. The error in approximating the interelectronic term can be estimated as

$$\frac{1}{|\boldsymbol{r}_2 - \boldsymbol{r}_1|} \approx \frac{1}{||\boldsymbol{r}_2| - |\boldsymbol{r}_1||} - \frac{|\boldsymbol{r}_1||\boldsymbol{r}_2|(1 - \cos\theta_{12})}{||\boldsymbol{r}_2| - |\boldsymbol{r}_1||^3} \,. \tag{6}$$

The last term of equation (6) was evaluated in 2D simulations for several typical trajectories near the frozen planetary orbit and it was found to be always smaller than $1/||\boldsymbol{r}_2| - |\boldsymbol{r}_1||$. By 'typical' we mean trajectories belonging to the FPA stability island [3] in 6D phase space.

Evidently, it is the full angular momentum $l_1 + l_2$ that is constant in this problem and can, in particular, be taken as zero. Even so, if the l_i remain small, we obtain an approximate 1D model by taking them as constant, where it is not necessary to regularize because of the repulsive centrifugal barriers. It is important to emphasize that the adoption

of (5) as a 1D model does not contradict the $Zee \rightarrow eZe \rightarrow Zee$ transition, since here $|r_i|$ is just the distance from the nucleus, whereas the transition occurs through the small but finite angular momentum. In the limit where both $l_i \rightarrow 0$, we obtain a sharp barrier at the origin with the dynamics very similar to that of the regularized model [5]. There is no impediment to precessions of the inner ellipse, the only constraint being that the outer electron moves along with the major axis. This description is confirmed by 2D numerical calculation, where it can be seen that θ_{12} in equation (6) is almost always close to zero, except when the inner electron is close to the perihelion of the ellipse. In this case, however, $||\boldsymbol{r}_2| - |\boldsymbol{r}_1||$ is maximum and also the passage through the perihelion is very fast. Therefore, it turns out that we can safely discard the last term in equation (6), as has indeed been checked by direct numerical computations.

If the motion starts in the eZe configuration, we should instead use the Hamiltonian

$$H_{eZe} = \frac{1}{2}(\Pi_1^2 + \Pi_2^2) - \frac{2}{|\boldsymbol{r}_1|} - \frac{2}{|\boldsymbol{r}_2|} + \frac{l_1^2}{2r_1^2} + \frac{l_2^2}{2r_2^2} + \frac{1}{|\boldsymbol{r}_2| + |\boldsymbol{r}_1|}\,. \tag{7}$$

If the angular momenta remain small, this 1D motion will approximate the full 2D motion in which there occur short $eZe \rightarrow Zee \rightarrow eZe$ transitions. In the limit where $l_i \rightarrow 0$, we again obtain close correspondence with the motion of the regularized model. However, in agreement with [5] we find that the motion described by Hamiltonian (7) leads to rapid self-ionization of the helium atom. Conversely, the motion in (5) is surprisingly stable, in view of the fact that this two-freedom Hamiltonian does not possess any obvious approximate constant of the motion. The invariant tori of this nearly integrable system are centred on a stable periodic orbit where the outer electron barely moves; hence the name *frozen planetary atom*. The inner electron, on the other hand, describes an approximately Kepler orbit. The frequency of this Kepler orbit increases slowly with l_i, in agreement with the 2D simulation.

Full 2D calculations reveal that the frozen planetary atom is long lived in comparison with the period of the orbit, but eventually decays. In figures 3 and 4 we present 2D simulations close to the frozen planetary atom configuration. When the maximum value of the electron angular momentum ($l_{\max}$) is large, i.e. near to $\sqrt{2}$ for energy $E = -1$, the system becomes unstable as shown in figure 5. One *ad hoc* way of accounting for the finite life of the frozen planetary configuration could be based on the argument that the eZe configuration is sampled for short intervals, so that we could mix

$$H = RH_{Zee} + TH_{eZe} \tag{8}$$

with $R + T = 1$ and T small. It is clear that, as T increases from 0, the motion gets more and more unstable, becoming completely chaotic as $T \rightarrow 1$.

The value of R (or T) would be evaluated in 2D simulation by

$$R = t_{\text{rhs}}/t_{\text{tot}} = (t_{\text{tot}} - t_{\text{lhs}})/t_{\text{tot}} = 1 - t_{\text{lhs}}/t_{\text{tot}} = 1 - T \tag{9}$$

where t_{rhs} is the average time that electron 1 spends on the right-hand side of the nucleus as in figure 1 (Zee configuration), t_{lhs} is the time it spends on the left-hand side (eZe configuration) and $t_{\text{tot}} = t_{\text{rhs}} + t_{\text{lhs}}$ is the total orbital period. The value of T (or R) can be calculated in an analytical form considering the two-body problem with $E = -1$ and the result is

$$T = (\arccos\sqrt{1 - l^2/2} - \sqrt{l^2/2(1 - l^2/2)})/\pi \tag{10}$$

where $\sqrt{l^2}$ is the angular moment for the two-body problem or, approximately, the square root of the average square angular momentum considered in 2D simulation. However, the motion under the Hamiltonian (8) autoionizes only when T is very large ($T \approx 0.6$), in contrast to the initial expectations. For the cases presented in figures 3 and 4 (see figure 3(c)

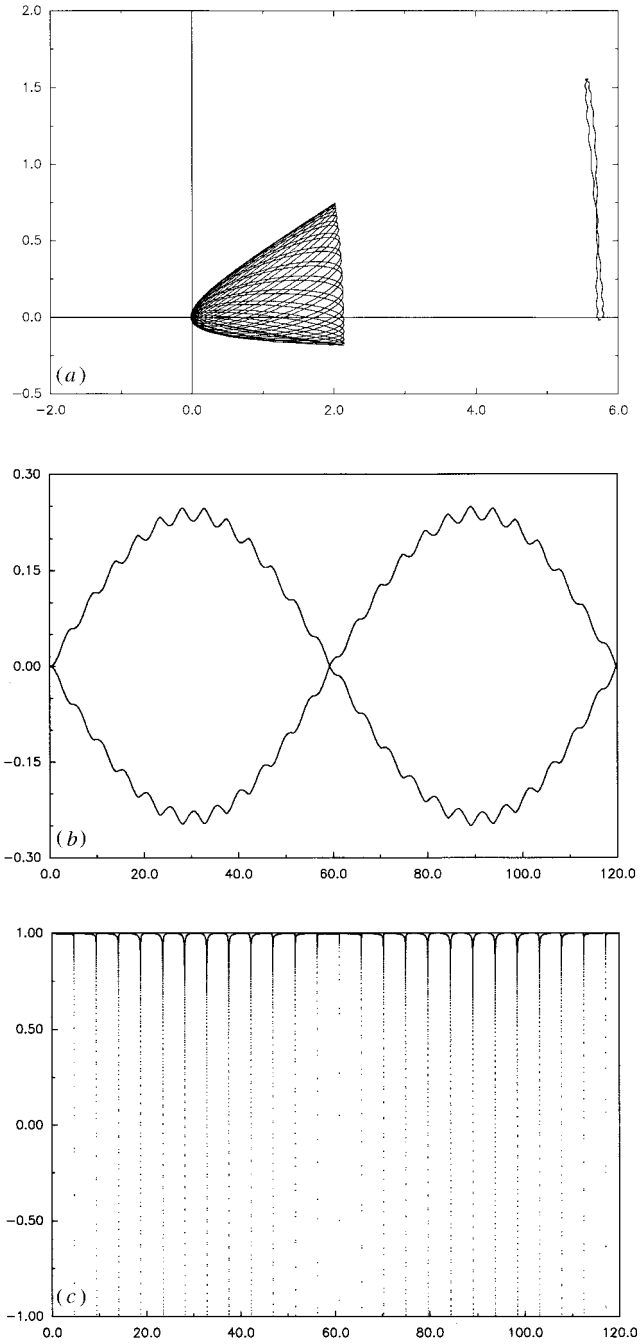

Figure 3. 2D helium atom simulation with total angular momentum $L = 0.0$ and $l_{\max} \approx 0.25$. (*a*) Trajectories of the electrons; (*b*) individual angular momenta l_i for each electron as a function of time: (*c*) cosine of the angle ($\cos\theta_{12}$) between the electron position vectors as a function of time (t_{rhs} can be evaluated for $\cos\theta_{12} > 0$ and t_{lhs} for $\cos\theta_{12} < 0$). The initial conditions of the trajectories are: $x_{\text{in}} = 0.000\,1350$, $y_{\text{in}} = -0.000\,01$, $p_{y\,\text{in}} = -12.698\,0597$, $E = -1.0$, $x_{\text{out}} = 5.7999$, $y_{\text{out}} = -0.0001$, $p_{x\,\text{out}} = 0.0001$ and $p_{y\,\text{out}} = 0.0$.

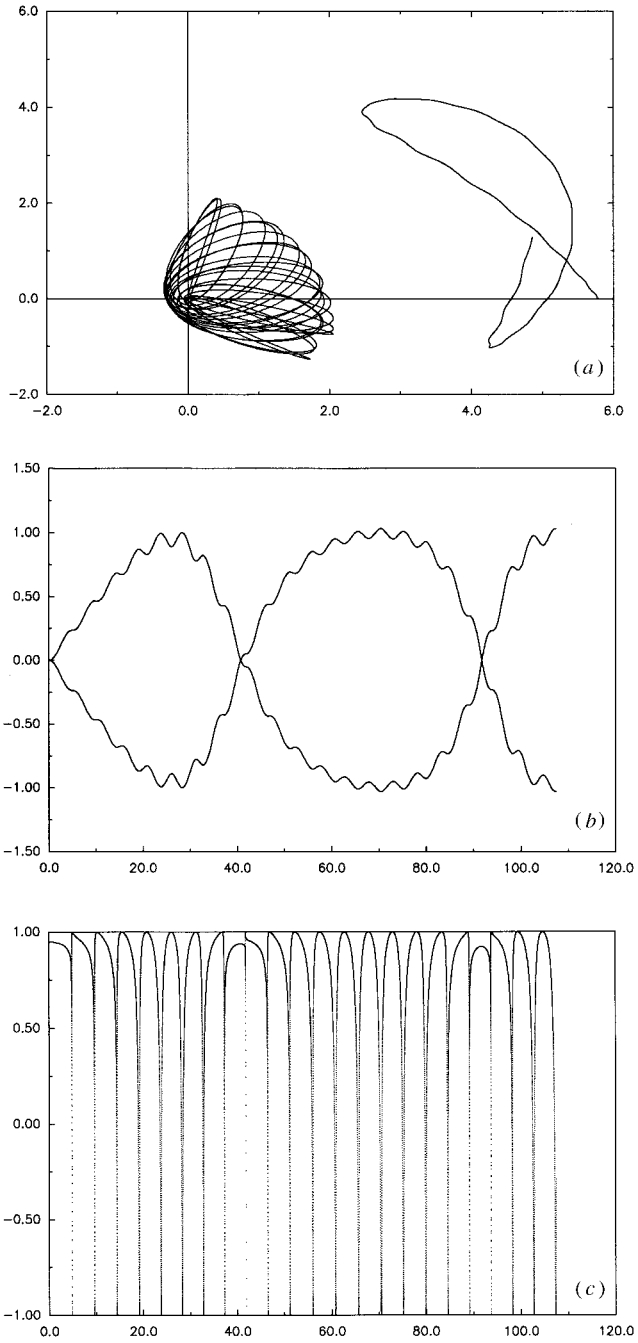

Figure 4. 2D helium atom simulation with total angular momentum $L = 0.0$ and $l_{\max} \approx 1.00$. (*a*) Trajectories of the electrons; (*b*) individual angular momenta l_i for each electron as a function of time: (*c*) cosine between the electron position vectors as a function of time. The initial conditions of the trajectories are the same as figure 3, except for $x_{\text{in}} = 0.000\,03$ and $p_{y\,\text{in}} = -112.467\,8292$.

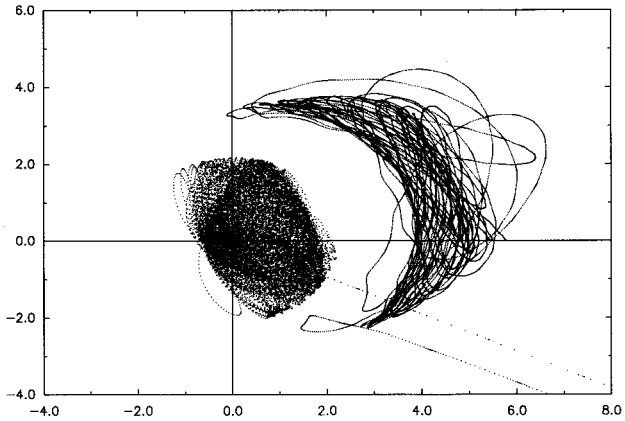

Figure 5. Trajectory of the 2D helium atom simulation with total angular momentum $L = 0.0$ and $l_{\max} \approx 1.28$. The initial conditions of the trajectory are the same as figure 3, but with $x_{\text{in}} = 0.000\,022$ and $p_{y\,\text{in}} = -168.352\,3413$.

and 4(c), in particular) we obtained $T = 0.000\,48$ and $T = 0.041$, respectively, which is much too small.

2.2. Time-dependent models

It is necessary, therefore, to attribute the finite lifetime of the frozen planetary atom to the variation of the individual angular momenta. Figures 3(b) and 4(b) display typical oscillations of the angular momenta for which

$$L = l_1(t) + l_2(t) = 0\,. \tag{11}$$

Estimating the variance $\overline{l_i^2} = l^2$ and the average frequency ω of these oscillations supplies the parameters for an approximate model where

$$l_1(t) = -l_2(t) = \sqrt{2}l \sin \omega t \equiv l_{\max} \sin \omega t\,. \tag{12}$$

At the cost of adding a periodic time dependence, we thus obtain a realistic 1D model

$$H_{Zee}(t) = \frac{1}{2}(\Pi_1^2 + \Pi_2^2) - \frac{2}{|\boldsymbol{r}_1|} - \frac{2}{|\boldsymbol{r}_2|} + l^2 \sin^2 \omega t \left(\frac{1}{r_1^2} + \frac{1}{r_2^2}\right) + \frac{1}{||\boldsymbol{r}_2| - |\boldsymbol{r}_1||}\,. \tag{13}$$

Fixing the energy as $E = -1.0$ au restricts $-\sqrt{2} \leqslant l_i(t) \leqslant \sqrt{2}$, where $l = \pm 1$ would describe the circular orbit limit.

The Kepler periods τ_k for the inner electron in the 2D and 1D models are approximately 4.69 au (l small) and 4.67 au, respectively. The precession frequency of the inner electron (or the orbital frequency of the outer electron) obtained from the average of the 2D numerical simulations is $\omega = 0.07$ au and we have used this value for the angular momentum oscillation frequency in the 1D model. This value of ω can be extracted from figures 3(b) and 4(b). The value $\omega = 0.07$ was obtained considering averages over FPA trajectories that were close to the autoionization limit. The variation of ω with $l_{\max}$ is in fact very small, being $\omega = 0.053$ for $l_{\max} \approx 0$ and increasing slowly until $\omega = 0.07$ near $l_{\max} \approx 1$. Figure 6 shows the stroboscopic map of a trajectory with initial conditions on the frozen planetary atom orbit of equation (13) for $l = 0.200$ (or $l_{\max} = 0.283$). Note that the outer electron oscillates for some time before the self-ionization.

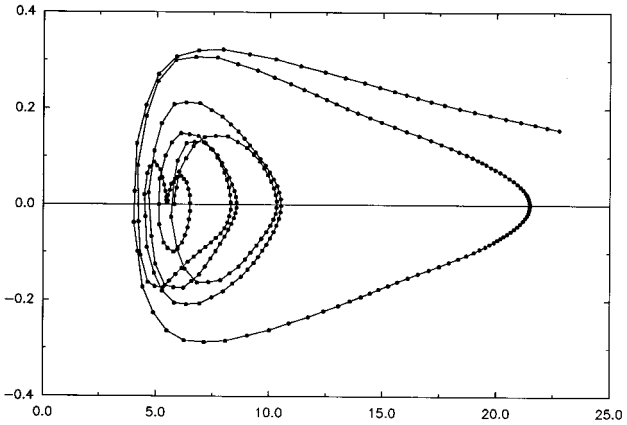

Figure 6. Poincaré map of the outer electron obtained via Hamiltonian (13) showing the self-ionization. The initial conditions of the trajectory are $r_1 = 0.000\,001$, $r_2 = 5.80$, $\Pi_2 = 0.0$, $E = -1.0$, $l_1 = -l_2 = 0.200$ ($l_{\max} = 0.283$) and $\omega = 0.07$.

Our careful heuristic derivation of the frozen planetary atom model (5) from the full 2D Hamiltonian has pointed the way to two possible modifications that account for its finite lifetime. Model (8) has the advantage of being strictly 1D, which will be helpful for subsequent discussion of semiclassical quantization, but is otherwise hard to justify. The time-periodic Hamiltonian (13) reduces the study of the frozen planetary atom regime to $2\frac{1}{2}$ freedoms, which is probably the simplest system in which the two electrons are considered explicitly, that we can realistically hope to deal with. In practice, the integration of Hamilton's equations under the Hamiltonian (13) presents some numerical difficulties, since the centrifugal term cannot be regularized. This is particularly cumbersome for small values of l, where numerical imprecision can lead to a false ionization. Our calculations show that for $l > 0.20$ the outer electron does ionize, although it is not easy to determine the precise value of l, say l_c, such that for $l < l_c$ the atom is stable.

2.3. Effective potential

There is yet the possibility for simplifying the description of the frozen planetary configuration if one is willing to discard the precise knowledge about the inner electron. This is the sort of treatment considered in the recent work by Shepelyansky [6] in which the effect of the inner electron is substituted by a time-averaged effective potential. This reduces the problem to just $1\frac{1}{2}$ freedoms. Following [6], we assume that the inner electron obeys the virial theorem

$$E = \langle V \rangle / 2 = -\langle T \rangle = -1/a \tag{14}$$

where the energy is equal to half the potential energy average ($\langle V \rangle$), T includes the linear momentum and the centrifugal term and a is the semi-major axis of the ellipse.

The time average of the interelectronic term $1/||\boldsymbol{r}_2| - |\boldsymbol{r}_1||$ that appears in equation (13) is

$$\frac{|\boldsymbol{r}_2|}{a\sqrt{r_2^2 - 2a|\boldsymbol{r}_2|}} - \frac{1}{a}\,. \tag{15}$$

Equation (13) can then be replaced by the effective ($1\frac{1}{2}$ freedoms) Hamiltonian

$$H_{Zee}(t) = \frac{1}{2}\Pi_2^2 - \frac{2}{|\boldsymbol{r}_2|} + \frac{l^2 \sin^2 \omega t}{r_2^2} - \frac{2}{a} + \frac{|\boldsymbol{r}_2|}{a\sqrt{r_2^2 - 2a|\boldsymbol{r}_2|}}\,. \tag{16}$$

In equation (16) we consider only very slow motions (precession), since the very fast movement has been integrated out.

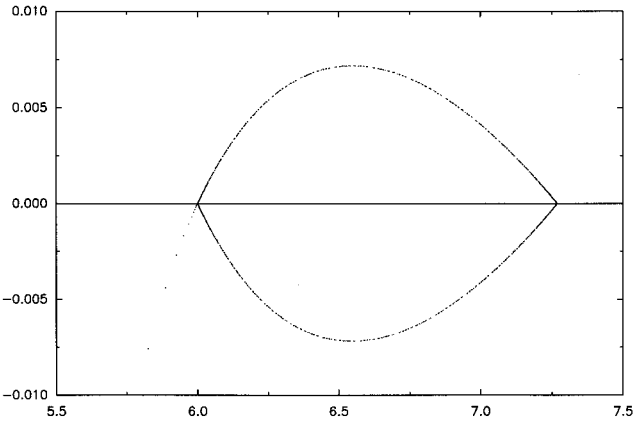

Figure 7. Poincaré map of the electron obtained via Hamiltonian (16) showing the self-ionization. The initial conditions of the trajectory are: $r_2 = 6.00$, $\Pi_2 = 0.0$, $E = -1.0$, $l_1 = -l_2 = 0.804\,221$ ($l_{\max} = 1.1373$), $a = 1.110\,118$ and $\omega = 0.07$.

The stroboscopic map of equation (16) is presented in figure 7, showing the system for $l_{\max} = 1.1373$, the lowest angular momentum for autoionization. This value for $l_{\max}$ is approximately the same as that found in 2D calculation. The goodness of this results shows that the frozen planetary atom configuration in one dimension is better described by an average potential produced by the nuclei inner-electron subsystem acting on the outer electron than by the approximation (3) which is equivalent to a Zee configuration.

3. Conclusion

The models analysed in this paper confirm the importance of the angular momentum variation for the instability of the frozen planetary atom. The model given by equation (8) also reinforces this conclusion, since, in that case, l is constant, and we obtain autoionization only for very high values of T. In these models there will still be a periodic orbit corresponding to the frozen planetary orbit for sufficiently weak perturbations (T in the case of (8) or l in (13) or (16)). This is guaranteed by the implicit function theorem (see, e.g., [7]). However, increasing the perturbations compromises the stability surrounding this orbit.

Acknowledgments

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