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CENTER MANIFOLD OF UNSTABLE PERIODIC ORBITS OF HELIUM ATOM: NUMERICAL EVIDENCE.

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Abstract. An original numerical method is introduced for the calculation of orbits on the center manifold of an unstable periodic orbit. The method is implemented for some unstable periodic orbits of the helium atom, and the dynamics on the corresponding center manifold is exhibited.

1. **Introduction.** This paper is devoted to a numerical study of the center manifold for some unstable periodic orbits, in a classical model of the helium atom. To this end an original method is introduced for the calculation of orbits on the manifold, which is of some interest in itself; then an implementation for the helium atom is given. Let us recall that the study of the classical model of the helium atom is of interest for the problem of the semiclassical limit of the corresponding quantum problem (see for example [1] and references therein); in particular the *stable* periodic orbits are used for an approximate estimate of the energy levels. On the other hand it was recently pointed out [2] that there is also a class of *unstable* periodic orbits which has a considerable relevance, namely the orbits having vanishing dipole moment, i.e. with the center of mass of the electrons fixed at the position of the nucleus. Indeed, it was shown (see [2] and also [3]) that the motions on the stable manifold of such unstable periodic orbits can provide tight emission lines, at variance with the common belief, that classical physics can provide only broad emission lines for atomic systems. In addition it was found that, provided some resonance conditions are satisfied, the lines thus computed agree rather well with some actually observed ones. In the quoted papers particular emphasis was also given to the possible existence and relevance of resonance islands located on the corresponding center manifold. But, due to the difficulties of a full analysis, the investigation was limited to the case of circular periodic orbits, i.e. orbits for which the relative distance between the two electrons remains constant while they revolve about the nucleus in phase opposition. In such a case it was possible to prove the existence of a center manifold and to compute analytically its dimension. But in the general case the problem of the very existence of the center manifold was left open, as was also the possible existence of a chaotic dynamics on it.

In the present paper a strong numerical evidence is given for the existence of the center manifold of a generic unstable periodic orbit, and the corresponding motions

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are illustrated. Notice that the numerical study of the center manifold in such a case is not at all a routine task. Indeed such orbits are unstable both for the forward flow and for the backward one (due to the hamiltonian character of the system), so that all algorithms using direct numerical integration fail. This situation is shared by other systems, for example the motions near the Lagrangian unstable equilibrium points in the restricted three body problem of celestial mechanics. In the literature (see [4]) one can find semi–analytic approaches where one tries to find an approximate analytical expression for the center manifold as the graph of a function of the form $y = f(x)$, $y \in \mathbb{R}^n$, $x \in \mathbb{R}^m$ (using an algebraic manipulator for high precision computations), and then the equations are numerically integrated using the constraint thus found.

In this paper we follow a different approach, introducing an original algorithm which is fully numeric, selects only the bounded orbits, and has the property that the center manifold becomes attractive for it. The method has been developed for dealing with the helium system, but we hope to implement it in the next future for Lagrangians of a more general type.

The paper is organized as follows: in Section 2 the problem of periodic orbits for the helium atom is posed, in Section 3 the algorithm is introduced and discussed, while some results are presented in Section 4.

2. **The periodic orbits.** The equations of motion for the helium system with $\mathbf{x}_1$, $\mathbf{x}_2$ denoting the positions in $\mathbb{R}^3$ of the two electrons and the nucleus being fixed at the origin, are:

$$\begin{aligned} m\ddot{\mathbf{x}}_1 &= -2e^2\frac{\mathbf{x}_1}{|\mathbf{x}_1|^3} + e^2\frac{\mathbf{x}_1-\mathbf{x}_2}{|\mathbf{x}_1-\mathbf{x}_2|^3} \\ m\ddot{\mathbf{x}}_2 &= -2e^2\frac{\mathbf{x}_2}{|\mathbf{x}_2|^3} + e^2\frac{\mathbf{x}_2-\mathbf{x}_1}{|\mathbf{x}_2-\mathbf{x}_1|^3} \ , \end{aligned} \tag{1}$$

where e and m are the charge and the mass respectively of the electron. Introducing as new variables twice the position of the center of mass $\mathbf{x} = \mathbf{x}_1+\mathbf{x}_2$ and the relative distance $\mathbf{r} = \mathbf{x}_1 - \mathbf{x}_2$, and choosing mass and charge units so that $m = 1$, $e^2 = 1$, one gets the equations

$$\begin{aligned} \ddot{\mathbf{x}} &= -8\frac{\mathbf{x}+\mathbf{r}}{|\mathbf{x}+\mathbf{r}|^3} - 8\frac{\mathbf{x}-\mathbf{r}}{|\mathbf{x}-\mathbf{r}|^3} \\ \ddot{\mathbf{r}} &= -8\frac{\mathbf{x}+\mathbf{r}}{|\mathbf{x}+\mathbf{r}|^3} + 8\frac{\mathbf{x}-\mathbf{r}}{|\mathbf{x}-\mathbf{r}|^3} + 2\frac{\mathbf{r}}{|\mathbf{r}|^3} \ , \end{aligned} \tag{2}$$

which can be deduced from the Lagrangian

$$\mathcal{L} = \frac{\dot{\mathbf{x}}^2}{4} + \frac{\dot{\mathbf{r}}^2}{4} + \frac{4}{|\mathbf{x}+\mathbf{r}|} + \frac{4}{|\mathbf{x}-\mathbf{r}|} - \frac{1}{|\mathbf{r}|} \ . \tag{3}$$

It is easy to check by direct inspection that $(\mathbf{x}(t), \mathbf{r}(t))$, with $\mathbf{x}(t) = 0$, and $\mathbf{r}(t)$ a bounded solutions of the Kepler problem $\ddot{\mathbf{r}} = -14\mathbf{r}/|\mathbf{r}|^3$, is a periodic solution of (2). In particular, circular motions $\mathbf{r}(t)$ of constant radius $|\mathbf{r}| = R_0$ give a periodic solution of period $T = 2\pi\sqrt{R_0^3/14}$. All these periodic orbits are characterized by having the electrons revolving about the nucleus in phase opposition.

The character of the invariant manifolds of the circular periodic orbits can be determined analytically, using a reference frame rotating with the same frequency of the periodic orbit. In such a frame a periodic orbit corresponds to a fixed point which can be studied by standard methods (see for example [3]); it can be

proved that such fixed points are unstable and possess a ten–dimensional center manifold. Instead, for the periodic orbits corresponding to elliptic motions of the relative distance $\mathbf{r}$ (elliptic periodic orbits for short), apparently nothing is known at an analytic level. Numerical evidence suggests that all these periodic orbits are unstable, because small perturbations of the initial data lead to self-ionization of the atom: after a small number of turns one of the electrons escapes to infinity, and the other one falls close to the nucleus. The most extensive computations in the literature are those of Kaneko [1], who was also able to detect some stable periodic orbits. But such periodic orbits are completely different from the ones studied here, inasmuch as they are characterized by great values of $\mathbf{x}$, while we concentrate to the case $\mathbf{x} \sim 0$. For what concerns the unstable elliptic period orbits, the dimension of their unstable manifold (and of the corresponding stable one, the system being conservative) is unknown, and is also unknown whether a center manifold exists at all. The present paper gives a strong numerical evidence that the stable and unstable manifolds are one–dimensional, and that there exists a ten-dimensional center manifold.

In the next section we describe the algorithm used to find the orbits on the center manifold.

3. **Numerical Algorithm.** Consider the first equation of system (2) (i.e. that for the center of mass), and split it into a part linear in $\mathbf{x}$, and a remainder of higher order, i.e. write it in the form

$$\ddot{\mathbf{x}} = \hat{A}(\mathbf{r})\mathbf{x} + \mathbf{R}(\mathbf{r}, \mathbf{x}) \ ; \tag{4}$$

where the matrix $\hat{A}(\mathbf{r})$ is defined by $A_{i,j}(\mathbf{r}) \stackrel{\text{def}}{=} \frac{16}{|\mathbf{r}|^5}(\delta_{i,j} - 3r_i r_j/|\mathbf{r}|^2)$, r_i being the i–th component of $\mathbf{r}$, and $\delta_{i,j}$ is the Kronecker symbol, while the expression for the remainder $\mathbf{R}$, obviously defined by $\mathbf{R} = \mathbf{F} - \hat{A}\mathbf{x}$, has no particular relevance.

To understand the essence of the method suppose that the relative motion $\mathbf{r}(t)$ and the remainder $\mathbf{R}(t)$ are given as explicit functions of time. In this case equation (4) turns out to be a linear one with time dependent coefficients.

Now, the bounded motions for a linear system can be studied by a technique similar to that used for obtaining the Lyapunov exponents for the same type of systems (see [5] and references therein). Indeed, it is well known (see [6]) that, given a linear system $\dot{\mathbf{v}} = \hat{B}(t)\mathbf{v} + \mathbf{f}(t)$ with suitable hypotheses on $\hat{B}(t)$ (the main one being that $\hat{B}(t)$ should be bounded), there exists an orthogonal transformation $\hat{H}(t)$ which brings the system into the form $\dot{\mathbf{z}} = \hat{T}(t)\mathbf{z} + \mathbf{h}(t)$, where $\hat{T}$ is upper triangular. In particular, the Lyapunov exponents are then given by $\lambda_i = \lim_{\tau\to\infty} \frac{1}{\tau}\int_0^\tau T_{ii}(t)\mathrm{d}t$.

Because of the Hamiltonian character of the original system, it happens that the exponents occur in opposite pairs, i.e. one has $\lambda_1, \ldots, \lambda_l, 0, \ldots, 0, \lambda_{n-l}, \ldots, \lambda_n$, with $\lambda_i > 0$ and $\lambda_{n-l+i} = -\lambda_i$, $i = 0, \ldots, l$ for a certain $l \le n/2$. When the system is put in upper triangular form, in order to find the stable motions one first integrates the last $n - l$ equations in an interval $[0, \tau]$ with a suitable sufficiently large τ (see below); from $T_{ij} = 0$ for $j < i$, one obtains for $i > l$

$$\dot{z}_i = \sum_{j\ge i} T_{ij}(t) z_j + h_i(t) \quad i = l+1, \ldots, n \ . \tag{5}$$

Having chosen an initial value $z_i(0)$, $i = l+1, \ldots, n$, these equations can be integrated numerically by any standard method, because the hard problem of having to deal with systems presenting positive Liapunov exponents, such as the original

one (4), has now been eliminated. Once the functions $z_i(t)$, $i > l$, are determined, to find the remaining z_i, $i = 1, \ldots, l$, one has to integrate the system

$$\dot{z}_i = \sum_{i \le j \le l} T_{ij}(t) z_j + \sum_{j>l} T_{ij}(t) z_j(t) + h_i(t) \ , \tag{6}$$

where in the r.h.s the terms containing $z_j(t)$, $j > l$, which are known on the interval $[0, \tau]$, have been put in evidence. The solutions of this system in general diverge exponentially as time increases, but the bounded solutions can be found by choosing some final value $z_i(\tau)$ and then integrating backward in time. If the integration interval $[0, \tau]$ is chosen sufficiently large with respect to the smallest positive Lyapuov exponent, the resulting trajectories would lie on the center manifold. We stress that the choice of the final data, as well as of the initial one on the stable manifold, is irrelevant, because such data are "forgotten" after a short transient. So, for example, they can be set to zero without practically affecting the resulting motion on the center manifold.

In our case the transformation $\hat{H}$ which puts the system into upper triangular form can be defined as follows. First, defining $\mathbf{v} \stackrel{\text{def}}{=} (\mathbf{x}, \dot{\mathbf{x}})$, $\mathbf{f} = (0, \mathbf{R})$ and $\hat{B}(\mathbf{r})$ as the matrix

$$\hat{B}(\mathbf{r}) = \begin{pmatrix} 0 & \mathbb{1} \\ \hat{A}(\mathbf{r}) & 0 \end{pmatrix} \ , \tag{7}$$

we put system (4) in the standard first order form $\dot{\mathbf{v}} = \hat{B}\mathbf{v} + \mathbf{f}$. Then, the matrix $\hat{H}$ is chosen as the solution of the non–linear differential equation

$$\dot{\hat{H}} = \hat{H}\hat{P} \ , \tag{8}$$

where we have defined (denoting by $\hat{H}^T$ the transpose of $\hat{H}$)

$$\hat{P}_{ij} \stackrel{\text{def}}{=} \begin{cases} (\hat{H}^T \hat{B} \hat{H})_{ij} & \text{if} \quad i > j \\ 0 & \text{if} \quad i = j \\ -P_{ji} & \text{if} \quad i > j \ , \end{cases} \tag{9}$$

and we take the identity matrix as initial data, i.e. take $\hat{H}_0 = \mathbb{1}$. It is apparent, from the very definition, that $\hat{P}$ is skew–symmetric, so that it follows that $\hat{H}$ will be orthogonal if orthogonal initial data are taken. Now, defining $\mathbf{z}$ through the relation $\mathbf{v} = \hat{H}\mathbf{z}$, system (4) turns out to be equivalent to

$$\begin{aligned} \dot{\mathbf{z}} &= \hat{T}\mathbf{z} + \hat{H}^T \mathbf{f} \\ \dot{\hat{H}} &= \hat{H}\hat{P} \ , \end{aligned} \tag{10}$$

with $\hat{T} \stackrel{\text{def}}{=} \hat{H}^T \hat{B} \hat{H} - \hat{P}$. But, from the definition of $\hat{P}$, it follows that $\hat{T}$ is upper triangular, and so we have performed the required transformatiom.

In our case there are two difficulties: first, the motion $\mathbf{r}(t)$, on which the matrix $\hat{A}$ in (4) depends, is not known in advance, but depends on $\mathbf{x}$ itself, so that it is impossible to perform this kind of two–steps integration. In addition, the remainder too depends on both $\mathbf{r}$ and $\mathbf{x}$. To overcome the problem we introduce an iterative procedure defining the functions $\mathbf{r}_n$ $\mathbf{x}_n$, $n = 0, 1, \ldots$, as solution of the system

$$\begin{aligned} \ddot{\mathbf{r}}_n &= \mathbf{G}(\mathbf{x}_{n-1}, \mathbf{r}_n) \\ \ddot{\mathbf{x}}_n &= \hat{A}(\mathbf{r}_n)\mathbf{x}_n + \mathbf{R}(\mathbf{x}_{n-1}, \mathbf{r}_n), \end{aligned} \tag{11}$$

where the function $\mathbf{G} \stackrel{\text{def}}{=} \frac{\partial \mathcal{L}}{\partial \mathbf{r}}$ is the r.h.s of the second equation of (2), while $\mathbf{R} = \frac{\partial \mathcal{L}}{\partial \mathbf{x}} - A(\mathbf{r})\mathbf{x}$ is the remainder in (4). It is clear that if the sequences $\mathbf{x}_n$, $\mathbf{r}_n$ converge

(in C^2 norm for example) to some limits $\mathbf{x}$, $\mathbf{r}$, the latter functions will be solutions of equation (2).

In this way the first equation of (11) decouples from the second one and they can be both solved independently. One starts with $\mathbf{r}_0 = 0$, $\mathbf{x}_0 = 0$ and numerically computes first $\mathbf{r}_1(t)$, which in any case coincides with a pure Kepler motion, because one has $\mathbf{G}(0, \mathbf{r}) = 7\mathbf{r}/|\mathbf{r}|^3$. Once $\mathbf{r}_1(t)$ is known as a function of time, the second equation of (11) reduces to a non–homogeneus linear equation; this, in turn, using the method described above, can be integrated to produce a solution $\mathbf{x}_1(t)$ which remains bounded over a large interval of time. Now the second approximation $\mathbf{r}_2(t)$ can be computed from the first equation of (11); here $\mathbf{G}(\mathbf{x}_1(t), \mathbf{r})$ is a known function depending on both t and $\mathbf{r}$. In addition, if one chooses small enough initial data for $\mathbf{x}_1$, then $\mathbf{G}(\mathbf{x}_1(t), \mathbf{r})$ differs only slightly from $7\mathbf{r}/|\mathbf{r}|^3$ because it depends quadratically on $\mathbf{x}_1$, so one will have that $\mathbf{r}_2(t)$ will differ slightly from $\mathbf{r}_1(t)$ (if one integrates over a finite interval of time, choosing the same initial conditions). The method can be iterated producing a sequence $\mathbf{x}_n$, $\mathbf{r}_n$ of bounded functions. The problem now consists in showing that the sequence $\mathbf{r}_n$, $\mathbf{x}_n$ converges; in any case, working at a numerical level, one can stop the iterations as usual, i.e. when the difference between two iterates is smaller than a preassigned accuracy.

We add here a further comment: when studying periodic orbits, one is often accustomed to compute the eigenvalues of the corresponding monodromy matrix, and one might like to understand the relation with the present method. In this connection we remark first of all that in our case the involved variational equation splits up into two disjoint equations, for the relative motion $\mathbf{r}(t)$ and for the variable $\mathbf{x}(t)$ respectively. Now the first equation is trivial, being the standard one for the Kepler problem. Thus only the second one is of interest, and is nothing but the linear part of the second equation of system (11), namely the one which we are actually studying. So, the computation of the eigenvalues of the monodromy matrix for a given periodic orbit, would just be obtained by performing the calculation described above for the corresponding particular initial data.

4. **Numerical results.** Let us first give some technical details. From the numerical point of view, the choice of the numerical integrator is irrelevant. The problem is rather that at every step the whole set of values of the functions $\mathbf{x}_n$, $\mathbf{r}_n$ have to be stored, so that memory can become a critical factor if one wants to find the orbit over a long interval of time. So it is convenient to choose methods which give good accuracy with large integration steps. To perform the integrations we used the standard Adams fourth order method, choosing the integration step of order of 10^{-4} to insure good conservation of total energy and angular momentum. We integrated orbits with initial data in the domain $1 \leq |r| \leq 1.5$ and $1 \leq |\dot{\mathbf{r}}| \leq 2$ for the relative distance, while the center of mass data were chosen in the domain $0 \leq |\mathbf{x}| \leq 0.01$ and $0 \leq |\dot{\mathbf{x}}| \leq 0.05$. Computations were performed both in double precision and in quadruple precision (always with the same integration step), and we checked that the method produces sequences which (appear to) converge if the integration interval $[0, \tau]$ is chosen not too large.

There appears to exist an upper time $\bar{\tau}$ such that, if one tries to integrate the equation for a longer time, the iterations do not converge anymore. If one increases the precision of computation, i.e one decreases the round–off error moving from double to quad precision for example, then this upper time $\bar{\tau}$ increases. As can be seen from table 1, it seems that this relation is of exponential type: to a doubling

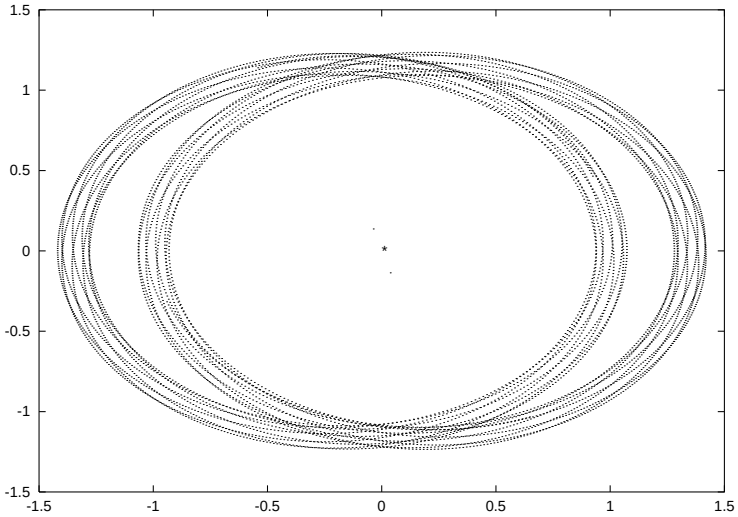

FIGURE 1. Orbit on the Center Manifold

of the precision there corresponds a doubling of the upper limit $\bar{\tau}$. The data in the table are given for an orbit with energy $E = 3$ and angular momentum $L = 2$. The times in the table are given in integration steps and correspond to some tenths of revolutions.

Type	Time
Double	4.10^5
Quad	7.10^5

TABLE 1. Maxmimum integration time

To obtain orbits for larger times one can proceed as follows: after computing the orbits on the interval $[0, \tau]$ (with $\tau \leq \bar{\tau}$) one stores the values for $\mathbf{x}$, $\mathbf{r}$ at some time t, say $t = 2\tau/3$, in such a way that one might be confident that the orbit stays on the center manifold. Then one uses these values as the initial ones for the computation of a new orbit. One can check (numerically) that the new orbit agrees with the older one in the common domain of definition so that the new orbit gives a real prolongation of the older one. Iterating this method, one can produce solutions stable on times of the order of hundreds of revolutions, and this has to be compared with the usual self–ionization times which correspond to few revolutions. In Figure 1 we report a plot of an orbit thus obtained, which corresponds to $E = 3.$, $L = 2.$, having $\mathbf{x}_0 = (0.1, 0)$ and $\dot{\mathbf{x}}_0 = (0.1, 0)$ as the center of mass initial data.

E	L	λ_1	λ_2	λ_3	λ_4
-3.00	2.0	1.861	0.003	-0.008	-1.856
-4.75	1.5	4.00	0.003	-0.02	-3.98

TABLE 2. Lyapunov Exponent

In Table 2 the Lyapunov exponents for the system (4) concerning the variable $\mathbf{x}$, for some orbits corresponding to different values of total energy E and total angular momentum L, are reported ; notice that the initial data correspond to generic periodic orbits, not to strictly circular ones. In the Table only four Lyapunov exponents are given, because the initial data for the positions and velocity of both electrons where chosen lying in a plane, so that the resulting motion is planar, and there are only four exponents. The reason for the choice of restricting the attention to planar motions is that in such a case the orbits of the complete system can be easily visualized through a suitable Poincaré map, as will be explained below. In any case, only one positive Lyapunov exponent is found, and this give strong evidence that, in the planar case, for every periodic orbit the center manifold is six–dimensional (as is analytically proven to be the case for the circular ones); indeed, in the planar case the phase space has dimension eight, and one remains with six dimensions when those related to the positive Liapunov exponent and to the corresponding negative one are dispensed with. The reason for the orbits on

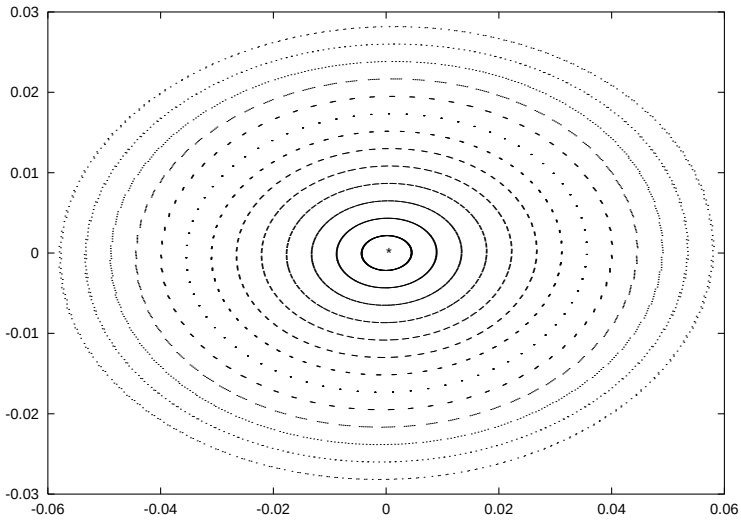

FIGURE 2. Poincaré Map

the center manifold actually lying on a three–dimensional manifold is as follows. For motions in a plane, the original phase space has dimension eight, which reduces to six due to conservation of angular momentum. Thus its intersection with the six-dimensional center manifold has dimension four (a greater dimension can only occur if the intersection is not transversal, which is not the case), and this reduces to three due to energy conservation. By a Poincaré section one is finally reduced to to a two-dimensional, easily visualizable, surface. In Figure 2 the Poincaré section is reported for some orbits which stay on the center manifold of the periodic orbit corresponding to $E = -3$ and $L = 2$. This figure seems to suggest that the orbits lie on smooth invariant curves.

If this were true, then the helium system would be integrable. One has however to remember that we are considering motions on the center manifold, and that the restriction of the system on this manifold has an elliptic periodic orbit. Now,

near such orbits Nekhoroshev theorem insures that chaos can be detected only on exponentially long times scale, and on the other hand our integration scheme, being non symplectic, is not suited for integrations over so long times (relative energy conservation is of order 10^{-5} after five hundred revolutions). So the problem remains open.

In conclusion, the numerical method presented here allowed us to obtain an interesting result for the dynamics of the helium atom, by producing evidence that a center manifold for some elliptic periodic unstable orbits might exist. Moreover the method allows also in principle to study the dynamics restricted to such center manifold, of which an example was given above.

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