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On the dynamics of the Langmuir problem

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Abstract
We study the dynamics of an invariant set of the classical Coulomb atom, which generalizes the one Langmuir proposed for helium in 1921. The n electrons are positioned at the vertices of a regular polygon that changes size homothetically, while the nucleus moves along a line orthogonal through the centre of the polygon. Our main result is that for negative energy the equations of motion have infinitely many periodic solutions.

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1. Introduction

In spite of explaining the spectrum of the hydrogen atom, Bohr's planetary model with Coulomb force failed to provide a good approximation for helium. But in 1921, Irving Langmuir (who would receive the Nobel Prize for chemistry in 1932) showed that if the electrons and the nucleus of the helium atom maintain an isosceles configuration while in motion, then the computed theoretical spectrum agrees with the measured one [L].

In this sense, an interesting mathematical problem is that of the qualitative study of Langmuir's model, i.e. that of the classical isosceles three-body problem (two electrons of equal masses and one nucleus, all assumed to be point particles) whose motion is generated by a Coulomb force. In this paper we will consider a model that contains Langmuir's as a particular case. We will study an $(n + 1)$-body problem ($n \geqslant 2$ electrons of equal masses and one nucleus). The electrons, which are at the vertices of a regular polygon, move homothetically in a fixed plane such that the polygon increases or decreases but does not change its shape, while the nucleus moves up and down on a line passing through the centre of the polygon and perpendicular to its plane. Since we are interested only in dynamical aspects, the point-particle hypothesis is reasonable. Obviously, for $n = 2$ we recover Langmuir's model. Like the isosceles problem, ours also has two degrees of freedom.

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The main goal of this paper is to come up with some new mathematical methods for finding periodic orbits in problems related to atoms. Our investigations are purely mathematical and we do not draw any physical conclusions. The model we present is general and our results work for a large class of parameters, including the ones interesting in physics, especially in semiclassical theory (see e.g. [RT, RW, TR]). To make physical sense, a model of the atom needs to satisfy certain minimal qualitative properties. A first condition is that the motion is bounded at least for a large class of solutions. (A uniform bound is better since it provides an estimate for the size of the atom.) Then we would also like to see that most solutions in this class are collisionless (which is not necessary but desirable). If these properties are satisfied, we can use some recurrence theorem to conclude that most solutions return infinitesimally close to any previous position. But the most important character of such a model would be that of having many periodic solutions. If periodic orbits exist, semiclassical theory can be used to compute the physical spectrum. In this paper we will show that our model, which generalizes that of Langmuir, has all the above-described qualitative properties.

In section 2 we derive the equations of motion and use them in section 3 to prove that every solution with negative energy $h < 0$ is bounded and that those with $h < h_0$, where $h_0 < 0$ is any fixed energy level, are uniformly bounded. In section 4 we regularize the equations of motion by the Levi-Civita method. This leads us to an analytic system that extends the collision solutions beyond singularities and is continuous with respect to initial data. In section 5 we rewrite the equations of motion in McGehee coordinates, which allow us to analyse the motion near total collision; this analysis is done in section 6. In section 7 we show that the system has four symmetries, which form a group isomorphic to that of Klein. This property allows us to show that the system cannot have equally symmetric periodic orbits. In section 8 we use the McGehee-type system and the Levi-Civita one to prove the existence of at least a finite number of nonhomothetic symmetric periodic orbits of our model. This result can be further used for testing the model within the framework of semiclassical theory. But of more importance seems to us the methodology we develop here, which can be applied to other dynamical systems for the detection of periodic orbits.

2. Equations of motion

Consider the Coulomb force acting on a unit-mass nucleus of charge +1 and on n electrons of mass m and charge $e < 0$. The electrons lie initially at the vertices of a regular polygon. The initial conditions are such that, within the plane of motion, the polygon shrinks or expands homothetically (changing size but preserving shape) and the nucleus moves on a vertical line perpendicular to the plane of the polygon (see figure 1). It is easy to see that this motion is well defined (i.e. that with respect to equations (1), written below, the above described set is invariant).

Let $\mathbf{q}_i$, $i = 1, \ldots, n$, be the position vectors and $\mathbf{p}_i = m\dot{\mathbf{q}}_i$, $i = 1, \ldots, n$, the momentum vectors of each electron, where the upper dot denotes the derivative with respect to the time t. Let $\mathbf{q}_{n+1}$ and $\mathbf{p}_{n+1} = \dot{\mathbf{q}}_{n+1}$ denote the position and momentum of the nucleus. Then $\mathbf{q} = (\mathbf{q}_1, \ldots, \mathbf{q}_{n+1})$ is the configuration of the system and $\mathbf{p} = (\mathbf{p}_1, \ldots, \mathbf{p}_{n+1})$ its momentum. In general (i.e. for any initial conditions except for those starting at collision) the motion of the nucleus and of the electrons forming the classical Coulomb atom is described by the Hamiltonian system

$$\begin{cases} \dot{\mathbf{q}} = \frac{\partial \mathbf{H}}{\partial \mathbf{P}}(\mathbf{q}, \mathbf{p}) \\ \dot{\mathbf{p}} = -\frac{\partial \mathbf{H}}{\partial \mathbf{q}}(\mathbf{q}, \mathbf{p}) \end{cases} \tag{1}$$

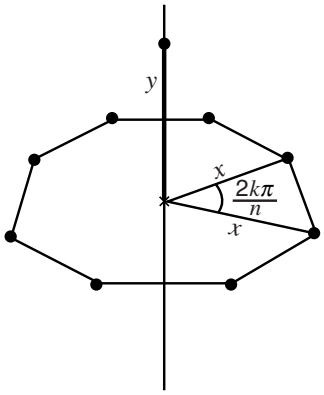

Figure 1. The electrons are at the vertices of a regular polygon that shrinks or expands homothetically, while the nucleus moves up and down on a line through the centre of the polygon and perpendicular to its plane.

where $H(\mathbf{q}, \mathbf{p}) = T(\mathbf{p}) + U(\mathbf{q})$ is the total energy $T(\mathbf{p}) = \frac{1}{2}\sum_{i=1}^{n} m^{-1}|\mathbf{p}_i|^2 + \frac{1}{2}|\mathbf{p}_{n+1}|^2$ is the kinetic energy and $U(\mathbf{q}) = \sum_{1\leqslant i<j\leqslant n} \frac{m^2e^2}{|\mathbf{q}_i-\mathbf{q}_j|} + \sum_{k=1}^{n} \frac{me}{|\mathbf{q}_k-\mathbf{q}_{n+1}|}$ is the potential energy. Since the dimension of the vector $(\mathbf{q}, \mathbf{p})$ is $6n + 6$, system (1) is $(6n + 6)$-dimensional.

In order to restrict our study to the above-described invariant set, we use as coordinates the vectors $\mathbf{x}_k = x\big(\cos\frac{2\pi k}{n}, \sin\frac{2\pi k}{n}, 0\big), k = 1, \ldots, n$, from the centre of the polygon to each of the electrons and the vector $\mathbf{y} = (0, 0, y)$ from the centre of the polygon to the nucleus (see figure 1). Note that $x \geqslant 0$ is the distance from the centre of the polygon to each electron and y is the distance (with sign positive if above the polygon, negative if below) from the centre of the polygon to the nucleus.

If we further denote $\mathbf{X} = (x, y), \mathbf{Y} = (P_x, P_y)$, where P_x and P_y are the conjugate momenta of x and y respectively, using some trigonometry we can show that equations (1) take the Hamiltonian form

$$\begin{cases} \dot{\mathbf{X}} = \frac{\partial \mathcal{H}}{\partial \mathbf{Y}}(\mathbf{X}, \mathbf{Y}) \\ \dot{\mathbf{Y}} = -\frac{\partial \mathcal{H}}{\partial \mathbf{X}}(\mathbf{X}, \mathbf{Y}) \end{cases} \tag{2}$$

where $\mathcal{H}(x, y, P_x, P_y) = \mathcal{T}(P_x, P_y) + \mathcal{U}(x, y)$ is the Hamiltonian function, $\mathcal{T}(P_x, P_y) = \frac{P_x^2}{2nm} + \frac{P_y^2}{2}$ is the kinetic energy and

$$\mathcal{U}(x, y) = \frac{nme}{(x^2 + y^2)^{1/2}} + \frac{nm^2e^2\gamma}{x}$$

denotes the potential energy, where $\gamma = \sum_{k=1}^{n-1} \frac{1}{4\sin\frac{k\pi}{n}}$ is a positive constant. Since the first term of the potential is negative (because $e < 0$) and the second one is positive, it becomes clear that the Coulomb force has an attractive component, exerted between the nucleus and each of the electrons, and a repelling one, acting among electrons. Note that system (2) is four dimensional, so the problem has two degrees of freedom.

The energy relation is

$$\frac{P_x^2}{2nm} + \frac{P_y^2}{2} + \frac{nme}{(x^2 + y^2)^{1/2}} + \frac{nm^2e^2\gamma}{x} = h \tag{3}$$

where h is the energy constant. In this paper we will be interested in negative values of h. As in [D-K], we can show that if $h \geqslant 0$ the solutions are unbounded, a case of no interest for the atomic model.

Note that the four equations of system (2), with variables constrained by the energy relation (3), lead to the study of a three-dimensional phase space. In the following sections we will show that the orbits that inhabit this three-dimensional phase space satisfy the properties described in the introduction.

3. Bounded and collisionless orbits

We will now prove that the only possible collision is the total one and that every solution with $h < 0$ is bounded. Moreover, if we fix any $h_0 < 0$, as close to 0 as we like, then all solutions with $h < h_0$ are uniformly bounded. In section 5 we will prove that the set of initial conditions leading to collisions is closed and negligible (in fact each negative energy level contains exactly one such solution) so except for those, all the other solutions are collisionless and bounded. In fact, for $h < h_0$ they are collisionless and uniformly bounded.

Theorem 1. *For equations (2), the only collision solutions are the ones ending in the simultaneous total collapse of all particles.*

Proof. This result is intuitively clear by the symmetry of motion and the form of the Coulomb force, which makes the electrons repel each other but attract the nucleus. The rigorous proof shows that if only some of the electrons collide, the symmetry is violated, so the only case to exclude is that of a simultaneous collapse of all electrons while the nucleus does not participate in the collision. That such a collision cannot take place is obvious from the energy relation (3). Indeed, when the orbits collide, the first two terms on the left-hand side are nonnegative (possibly infinite), the third term is negative but bounded, while the fourth term is infinite, so the left-hand side is infinite. The right-hand side, however, is a negative constant. The fact that the total collision between the nucleus and the electrons does take place under certain circumstances will become clear in section 6 (theorem 4) when we will find all solutions with this property. We will show there that they appear only if the nucleus is fixed at the centre of the polygon and that the electrons move homothetically until they simultaneously hit it. □

Theorem 2. *For $h < 0$, every solution of equations (2) is bounded. Moreover, for every $h_0 < 0$ fixed, the set of solutions with $h < h_0$ is uniformly bounded in phase space by a bound that depends on h_0.*

Proof. Let $h_0 < 0$ be fixed, then for all $h < h_0$, it is obvious from the energy relation (3) that $\mathcal{U}(x, y) \leqslant h < 0$. Using once again the energy relation, we can further derive the inequality

$$\frac{nme + nm^2e^2\gamma}{(x^2 + y^2)^{1/2}} \leqslant \mathcal{U}(x, y) \leqslant h < h_0$$

which implies that

$$(x^2 + y^2)^{1/2} \leqslant \frac{nme + nm^2e^2\gamma}{h} \leqslant \frac{nme + nm^2e^2\gamma}{h_0}. \tag{4}$$

Since the number n of electrons is between 2 and 111, a numerical computation shows that $0.25 < \gamma < 18$ (recall that $\gamma = \sum_{k=1}^{n-1} \frac{1}{4 \sin \frac{k\pi}{n}}$). For the hydrogen atom, the mass of the nucleus is 1836 times larger than that of the electron (in terms of the mass of ^{12}C taken as unity). For all the other atoms the mass of the nucleus is much larger than that of the electrons, so $nme + nm^2e^2\gamma$ is always negative. Since $h < 0$, the right-hand side of relation (4) is positive. But $(x^2 + y^2)^{1/2}$ is a measure of the particles' distribution in space, so the conclusions of the theorem follow from inequality (4). □

The classical recurrence theorem of Poincaré now yields the following conclusion, which mainly states that for $h < 0$ the solutions of system (2) are either periodic or quasiperiodic.

Theorem 3. *Except for a set of Lebesgue measure zero, every initial condition leads to a solution of system (2) that comes infinitely many times infinitesimally close to its initial condition.*

But of course, our main goal is to find periodic solutions. The above result does not guarantee their existence. They are the ones that, in the view of today's development of physics, can provide an explanation of the atoms' spectrum. To prove the existence of periodic orbits, we need to get into some technical mathematical details that will help us understand the motion of particles in the neighbourhood of collisions. As we will see later on, many of the solutions passing close to collision are periodic.

4. Levi-Civita regularization

Let us note that system (2) is singular at the total collapse and that this is its only singularity. In other words, when a total collision occurs, equations (2) lose their meaning, so they give us no information on the dynamical behaviour of the motion at and beyond the collision instant. To overcome this inconvenience, we can employ a *regularization* technique, which eliminates the singularity by analytically extending all collision solutions beyond collisions.

One of these regularization techniques was proposed by Tulio Levi-Civita in 1920 (see [LC]). The idea of this method is to consider some coordinate and time transformations that change system (2) into a new, equivalent, and free of singularities one. In the new system, the collision solutions are analytic at the instant of collision. Moreover, the new equations have the continuity property with respect to initial conditions, i.e., nearby solutions behave similarly on finite time intervals.

Let us remark that not all regularization techniques attract both properties, some leading only to an analytic continuation without continuity with respect to initial conditions or the other way around. Of course, the possibility of applying a certain regularization technique depends on the nature of the system, fortunately the Levi-Civita method applies to equations (2) as we now show in the remaining part of this section.

From the original Hamiltonian in variables (x, y, p_x, p_y) we can explicitly write the Hamiltonian system as

$$\begin{cases} \dot{x} = \frac{p_x}{nm} \\ \dot{y} = p_y \\ \dot{p}_x = \frac{nmex}{(x^2+y^2)^{3/2}} + \frac{nm^2e^2\gamma}{x^2} \\ \dot{p}_y = \frac{nmey}{(x^2+y^2)^{3/2}} \end{cases} \tag{5}$$

where the energy relation has the form

$$h = \frac{p_x^2}{2nm} + \frac{p_y^2}{2} + \frac{nme}{(x^2+y^2)^{1/2}} + \frac{nm^2e^2\gamma}{x^2}.$$

Let us observe that if $y \equiv 0$ and $p_y \equiv 0$ then $\dot{y} = 0$ and $\dot{p}_y = 0$, therefore the plane $\Pi = \{x, y = 0, p_x, p_y = 0\}$ is invariant under the flow given by the above system, which in the plane Π takes the form

$$\begin{cases} \dot{x} = \frac{p_x}{nm} \\ \dot{p}_x = \frac{nme}{x^2} + \frac{nm^2e^2\gamma}{x^2} = \frac{k}{x^2} \end{cases} \tag{6}$$

where $k = nme + nm^2e^2\gamma$, a quantity that is always negative under our hypotheses.

Consider now the Levi-Civita symplectic transformation given by

$$x = \xi^2 \qquad p_x = \eta\xi^{-1}$$

and let us apply it on the above Hamiltonian system. The time reparametrization $\frac{dt}{ds} = 2\xi^2$ then leads to the new system

$$\begin{cases} \xi' = \frac{\eta}{nm} \\ \eta' = 2h\xi \end{cases} \tag{7}$$

which we obtained with the help of the energy relation

$$2\xi^2 h = \eta^2 + 2k.$$

Note that for $h < 0$, equation (7) represents a harmonic oscillator; this implies that the motion can be analytically continued beyond collision. In other words, within the invariant set Π, the solution of the system has been regularized.

Let us now analyse the entire vector field in coordinates (ξ, y, η, p_y). Using the energy relation

$$2h\xi^2 = \frac{\eta^2}{nm} + p_y^2\xi^2 + \frac{2nme\xi^2}{(\xi^4 + y^2)^{1/2}} + 2nm^2e^2\gamma$$

we obtain

$$\begin{cases} \xi' = \frac{\eta}{nm} \\ y' = 2\xi^2 p_y \\ \eta' = 2h\xi - p_y^2\xi - \frac{2nme\xi}{(\xi^4+y^2)^{1/2}} + \frac{2nme\xi^5}{(\xi^4+y^2)^{3/2}} \\ p_y' = \frac{2nmey\xi^2}{(\xi^4+y^2)^{3/2}}. \end{cases} \tag{8}$$

Note that η and ξ cannot be simultaneously zero since such values do not satisfy the energy relation, therefore the above system is analytic everywhere and lacks equilibrium solutions. This proves that the total collision is regularizable on each negative energy level, i.e., the motion can be analytically extended beyond all collision singularities, and that continuity with respect to the initial conditions is present in system (8).

We will use these convenient properties of equations (8) in section 8. Until then we need to prepare the stage for proving the existence of certain types of periodic solutions, and we start by introducing some new coordinates.

5. McGehee coordinates

In this section we will perform some transformations (first considered by McGehee in a problem of celestial mechanics, see [M], [D]), which will allow us to understand the qualitative properties of the motion near total collision. The idea is to blow up the total collision singularity into what we will call a *collision manifold*. It will turn out that this collision manifold is topologically equivalent (i.e. it can be continuously deformed) to a two-dimensional sphere, which we will 'paste' to the phase space. Though the flow on this sphere has no physical meaning, its study will allow us to understand what happens to orbits passing close to collision in phase space. This is possible due to the continuity of the solutions with respect to initial conditions.

Let $\mathbf{A}$ denote the matrix

$$\mathbf{A} = \begin{pmatrix} nm & 0 \\ 0 & 1 \end{pmatrix}$$

and consider the transformations

$$\begin{cases} r = (\mathbf{X}^T \mathbf{A} \mathbf{X})^{1/2} \\ \mathbf{s} = r^{-1}\mathbf{X} \\ w = \mathbf{Y}^T \mathbf{s} \\ \mathbf{z} = \mathbf{A}^{-1}\mathbf{Y} - w\mathbf{s}. \end{cases}$$

Note that r is similar to the moment of inertia and therefore offers a measure of the particles' distribution in space, $\mathbf{s}$ is a rescaling of the configuration, w is the radial component of the momentum and $\mathbf{z}$ is the tangential one. Since r and w have dimension 1, whereas $\mathbf{s}$ and $\mathbf{u}$ have dimension 2, it means that the transformation is given by six relations. System (2) however is four dimensional, so the variables r, $\mathbf{s}$, w and $\mathbf{z}$ must be connected by two relations. Indeed, these relations are

$$\mathbf{s}^T \mathbf{A} \mathbf{s} = 1 \qquad \text{and} \qquad \mathbf{z}^T \mathbf{A} \mathbf{s} = 0.$$

By further rescaling w and $\mathbf{z}$, through

$$\begin{cases} v = r^{1/2} w \\ \mathbf{u} = r^{1/2} \mathbf{z} \end{cases}$$

and by using the time-rescaling transformation

$$\mathrm{d}\tau = r^{-3/2}\,\mathrm{d}t$$

system (2) becomes

$$\begin{cases} r' = rv \\ \mathbf{s}' = \mathbf{u} \\ v' = \mathbf{u}^t A \mathbf{u} + \frac{1}{2}v^2 + \mathcal{U}(\mathbf{s}) \\ \mathbf{u}' = -\frac{1}{2}v\mathbf{u} - (\mathbf{u}^t A \mathbf{u})\mathbf{s} - \mathcal{U}(\mathbf{s})\mathbf{s} - A^{-1}\nabla\mathcal{U}(\mathbf{s}). \end{cases}$$

Note that τ is the new (fictitious time) independent variable and that a prime now denotes the derivative with respect to τ. The above system is globally defined, i.e. every solution makes sense for all real values of τ.

In these new coordinates, the energy relation takes the form

$$\tfrac{1}{2}(\mathbf{u}^T \mathbf{A} \mathbf{u} + v^2) + \mathcal{U}(\mathbf{s}) = rh.$$

Further considering the transformations

$$\mathbf{s} = \mathbf{B}\begin{pmatrix} \cos\theta \\ \sin\theta \end{pmatrix} \qquad \mathbf{u} = u\mathbf{B}\begin{pmatrix} -\sin\theta \\ \cos\theta \end{pmatrix}$$

where

$$\mathbf{B} = \begin{pmatrix} (nm)^{-1/2} & 0 \\ 0 & 1 \end{pmatrix}$$

the above equations become

$$\begin{cases} r' = rv \\ \theta' = u \\ v' = u^2 + \frac{1}{2}v^2 + U(\theta) \\ u' = -\frac{1}{2}vu - \frac{\mathrm{d}}{\mathrm{d}\theta}U(\theta) \end{cases} \tag{9}$$

with

$$U(\theta) = (nm)^{3/2} e \left(\frac{1}{\sqrt{1 - (1 - nm)\sin^2\theta}} + \frac{me\gamma}{\cos\theta} \right)$$

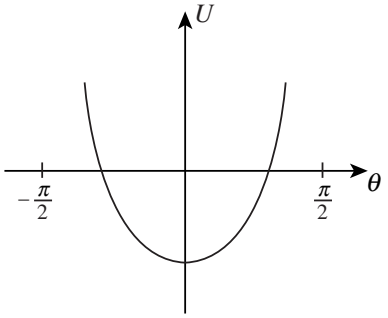

Figure 2. The graph of U for a choice of the parameters within the limits of the atom model. Note that the shape of the graph and the vertical asymptotes $\theta = -\frac{\pi}{2}$ and $\theta = \frac{\pi}{2}$ are independent of those values of the parameters that make sense for the atom model.

whose graph is as in figure 2. The energy relation takes the form

$$\tfrac{1}{2}(u^2 + v^2) + U(\theta) = rh. \tag{10}$$

Note that unlike equations (2), system (9) makes sense at total collapse (i.e. at $r = 0$). Since the above transformations are analytic diffeomorphisms from the domain of system (2) to the domain of system (9) minus the set of solutions for which $r = 0$, system (9) is analytic. The analyticity of (9), however, now extends to $r = 0$, which forms an invariant manifold that we pasted to the phase space. In the next section we will give to this manifold a geometric interpretation and show that it is fundamental for understanding the flow.

6. Collision orbits

We now proceed with the study of system (9), which will reveal several properties for collision and near-collision orbits. In this section we will define the collision manifold, show that the flow on it is increasing with respect to the variable v and prove that the only collision orbits are the homothetic ones.

In the previous section we saw that the singularities of system (2) correspond in system (9) to $r = 0$. It is then natural to look at what happens to every energy level at $r = 0$. From (10) we see that the energy relation becomes

$$u^2 + v^2 = -2U(\theta).$$

This means that all energy levels intersect along the manifold

$$C = \{(r, \theta, v, u) \mid r = 0 \text{ and } u^2 + v^2 = -2U(\theta)\}$$

which—according to the first equation of (9)—is an invariant set (i.e. a union of orbits). For obvious physical reasons, we will call C the collision manifold of system (9). Because of the shape of U (see figure 2), C is topologically equivalent (i.e. it can be continuously deformed) to a two-dimensional sphere (see figure 3). We can now prove the following result.

Lemma 1. *System (9) has two equilibria,* $N = (0, 0, \sqrt{-2U(0)}, 0)$ *and* $S = (0, 0, -\sqrt{-2U(0)}, 0)$*, and both belong to the collision manifold C.*

Proof. Obviously N (the north pole) and S (the south pole) are equilibria. To show that they are the only ones, we need to prove that $\frac{\mathrm{d}}{\mathrm{d}\theta}U(\theta) = 0$ has only the root $\theta = 0$. Since

$$\frac{\mathrm{d}}{\mathrm{d}\theta}U(\theta) = (nm)^{3/2} e \sin\theta \left(\frac{(1 - nm)\cos\theta}{[1 - (1 - nm)\sin^2\theta]^{3/2}} + \frac{me\gamma}{\cos^2\theta} \right)$$

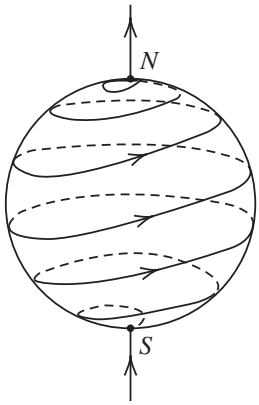

Figure 3. The flow on the collision manifold C and near the equilibria N and S.

the equation $\frac{\mathrm{d}}{\mathrm{d}\theta}U(\theta) = 0$ has solutions if $\sin\theta = 0$ (which implies $\theta = 0$ for $-\frac{\pi}{2} < \theta < \frac{\pi}{2}$) or for those θ that verify the equation

$$(1 - nm)\cos^3\theta = me\gamma[1 - (1 - nm)\sin^2\theta]^{3/2}.$$

But θ belongs to the interval $\left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$, so $\cos\theta > 0$ and $e < 0$. Since $2 \leqslant n \leqslant 111$ and $0 < m \leqslant \frac{1}{1836}$ mass units, the left-hand side of the above equation is always positive. But the right-hand side is always negative, so the above equation has no solutions. This completes the proof. □

We can now determine the behaviour of the flow on and near the collision manifold C in phase space. Let us prove the following result.

Lemma 2. *The flow on the collision manifold C is nondecreasing with respect to the variable v and every nonequilibrium orbit connects the south pole S with the north pole N. Moreover, on the collision manifold C, S is a spiral source and N is a spiral sink, whereas outside C, S has a one-dimensional stable manifold and N a one-dimensional unstable one.*

Proof. From the third equation of system (9) and from the energy relation (10) with $r = 0$, we find that $v' = \frac{1}{2}u^2$, so the flow is nondecreasing with respect to the variable v. To prove the rest of the theorem, we use the linearization method. The linear system around each of the two equilibria is given by the matrix

$$\begin{pmatrix} \pm\sqrt{-2U(0)} & 0 & 0 & 0 \\ 0 & \pm\sqrt{-2U(0)} & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & -\frac{\mathrm{d}^2}{\mathrm{d}\theta^2}U(0) & \mp\sqrt{-U(0)/2} \end{pmatrix}$$

with the upper sign for N and with the lower one for S. The first two eigenvalues are $\lambda_1 = \lambda_2 = \pm\sqrt{2U(0)}$, while λ_3 and λ_4 are the roots of the equation

$$\lambda^2 \pm \sqrt{-2U(0)}\lambda + \frac{\mathrm{d}^2}{\mathrm{d}\theta^2}U(0) = 0$$

whose discriminant, $\Delta = -2U(0) - 4\frac{\mathrm{d}^2}{\mathrm{d}\theta^2}U(0)$, is negative in the case of atoms (i.e. for $1 \leqslant n \leqslant 111$ and $0 < m \leqslant \frac{1}{1836}$ mass units). If we fix an energy level h, then we can work with the variables v, θ and u; the coordinate r is obtained directly from the energy relation (10),

more precisely, N has a one-dimensional unstable manifold (outside C) and a two-dimensional stable one (on C), so N is a spiral sink on C, whereas S has a one-dimensional stable manifold (outside C) and a two-dimensional unstable one (on C), so it is a spiral source on C. This completes the proof. □

Remark. Note that every orbit on C (except N and S, which are stationary) increases with respect to the variable v except at points with $u = 0$. This follows from the fact that for $r = 0$, $v' = \frac{1}{2}u^2$.

Before stating our next result, let us define a *homothetic orbit* as being a planar solution for which the nucleus lies at the centre of the regular polygon formed by the electrons, which simultaneously move towards or away from the nucleus such that the polygon dilates or contracts without changing shape. A homothetic orbit lies in the invariant set $\theta = u = 0$, which means that only the variables r and v change in time. From the above mathematical results we can now draw the following physical conclusions.

Theorem 4. *For every $h < 0$ there is only one homothetic orbit. Every such orbit starts from and ends in a total collision. No other orbits encounter collisions.*

Proof. To encounter a collision, an orbit must reach the collision manifold C. But due to the structure of the flow on and near C, the only way an orbit can end in a collision is if it reaches the south pole S. Similarly, the only way an orbit can emerge from a total collision is if it starts at the north pole N. Since for $h < 0$ every solution is bounded and since the set $\theta = u = 0$ is invariant for system (9), a homothetic orbit that starts at N must end in S. But since both the unstable manifold of N and the stable manifold of S are one-dimensional, the only orbits encountering collisions are the homothetic ones. This completes the proof. □

7. Symmetric solutions

Before finding more physical properties, we need to describe the symmetries of system (9) and to understand their algebraic structure. The first symmetry we put into evidence is the reversibility of the system, given by

$$S_0(r, \theta, v, u, \tau) = (r, \theta, -v, -u, -\tau)$$

which shows that for every solution there is another one that has the same position coordinates, and opposite velocities, all in reversed time. Another symmetry is given by

$$S_1(r, \theta, v, u, \tau) = (r, -\theta, v, -u, -\tau)$$

which implies that for every solution there is another one with opposite θ and u coordinates. And finally there is the symmetry

$$S_2(r, \theta, v, u, \tau) = (r, -\theta, -v, u, -\tau)$$

which means that for every solution there is another one with opposite coordinates θ and v in reversed time. Together with the composition of functions, denoted by $\circ$, and the identity

$$I(r, \theta, v, u) = (r, \theta, v, u),$$

these symmetries form a commutative group in which the operation acts according to the table below,

$\circ$	I	S_0	S_1	S_2
I	I	S_0	S_1	S_2
S_0	S_0	I	S_2	S_1
S_1	S_1	S_2	I	S_0
S_2	S_2	S_1	S_0	I

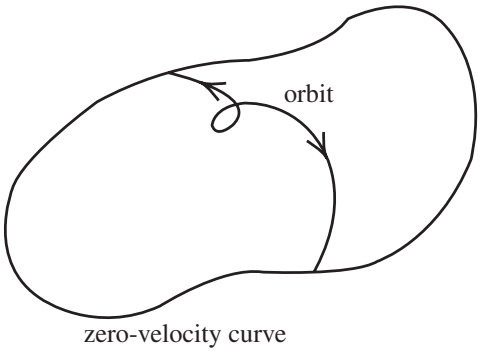

Figure 4. If a solution intersects the zero-velocity set (which in our problem is the θ-axis) at two distinct points, then the reversibility of the flow given by the symmetry S_0 implies that the solution is periodic. From the physical point of view the particles move from some rest position to another zero-velocity configuration and then return to the initial rest position, thus completing one period. Our figure is considered in the configuration space.

All these allow us to draw the following conclusion, whose proof is obvious from the above table.

Lemma 3. *The group of symmetries acting on system (9) is isomorphic with the group of Klein.*

We can now use the above symmetries to draw some conclusions about the non-existence of certain types of periodic orbits. Let us first note that the points for which $u = v = 0$ form a *zero-velocity set*. At the instant when a solution reaches this set, the nucleus and the electrons are at rest. The symmetry S_0 implies that if a solution touches the zero-velocity set at two distinct points, then it must be periodic (see figure 4). Such solutions are called *symmetric periodic*. In section 8 we will prove that the Langmuir problem has many periodic orbits of this kind.

A solution for which the two distinct points at which it touches the zero-velocity curve are $(r^*, \theta^*, 0, 0)$ and $(r^*, -\theta^*, 0, 0)$, with $r^*, \theta^* > 0$, is called *equally symmetric periodic*. The reason for introducing this terminology is that the two points are equally distanced from the origin of the coordinate system. From the physical point of view these solutions start from some nonplanar rest position, then move such that the nucleus reaches at rest a symmetric position with respect to the plane of the electrons, while the electrons come back to rest at the initial position. Then all the particles get back to the initial position, thus completing one period. Note that the homothetic solutions are not equally symmetric since in their case $\theta \equiv 0$. We can now prove the following result.

Theorem 5. *System (9) has no equally symmetric periodic solutions.*

Proof. Let us assume that an equally symmetric periodic solution exists (see figure 5). Then the points $(r^*, \theta^*, 0, 0)$ and $(r^*, \theta^*, 0, 0)$, with $r^*, \theta^* > 0$, belong to the solution. In order to analyse how the symmetries determine the shape of this orbit, we decompose it in the clockwise oriented arcs AB, BC and CA, as shown in figure 5.

The symmetry S_0 implies that the arcs AB and BC have the same θ and opposite u and v coordinates when travelling along AB in direct time (i.e. as the arrow points) and along BC in reversed time. The symmetry S_1 implies that, when followed along in direct time, the arcs AC

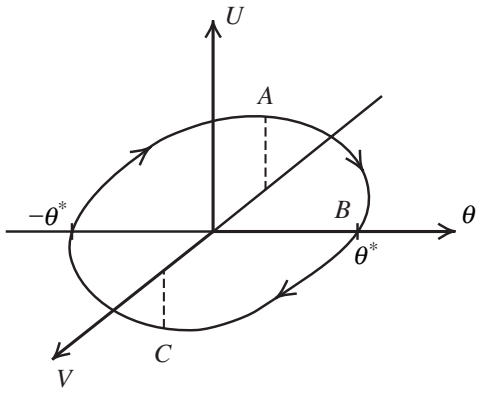

Figure 5. Because of the group of symmetries acting on the solutions of system (9), any equally symmetric periodic orbit must intersect the v-axis, which represents the homothetic solution. This intersection contradicts the uniqueness property, so equally symmetric periodic orbits cannot exist.

and CA have opposite θ and v coordinates and the same u coordinate. But while the condition on the θ and v coordinates is satisfied, the one on u works only if $u = 0$.

All these imply that the orbit must intersect the v-axis, i.e. at some point in time, $\theta = u = 0$. But $\theta = u = 0$ is the invariant set of the homothetic orbits, so the intersection cannot take place without violating the uniqueness property for the corresponding initial value problem of system (9). This contradiction shows that equally symmetric orbits do not exist. □

8. Nonhomothetic periodic orbits

In this section we will prove the existence of at least a finite number of nonhomothetic periodic orbits on each negative energy level. In phase space, these orbits lie in the neighbourhood of the homothetic solutions: the electrons oscillate homothetically between a close collapse and an outer limit dictated by the energy level, while the nucleus oscillates very slightly through and near the plane of the electrons. To show the existence of these orbits, we will use both systems (8) and (9). We are now going to prove the following result.

Theorem 6. *For each negative energy level, system (9) has infinitely many periodic orbits, out of which at least a finite number are symmetric and non-homothetic.*

Proof. Let us fix $h < 0$ and start with a straight segment Z_0 of initial conditions as shown in figure 6: Z_0 is contained in the zero-velocity curve and contains the initial condition that leads to the homothetic solution connecting N with S. Starting at time $\tau = 0$, the segment Z_0 follows the flow until, very close to the south pole S, it turns into a segment Z_1 at time τ_1. Since the flow on the collision manifold C has an infinite twist near S, the continuity with respect to initial data allows us to conclude that the closer to S, the more twisted Z_1 must be. In fact it may have an infinite twist, but only a finite one is guaranteed.

Since by analytically diffeomorphic transformations the equations (9) and (8) are equivalent, the segment Z_0 at time $\tau = 0$, which belongs to the flow of system (9), corresponds to a segment L_0 at time $s = 0$ of system (8); also the segment Z_1 at time τ_1 corresponds to a segment L_1 at time s_1. We now use system (8) to extend the segment L_1 to a segment L_2 at time

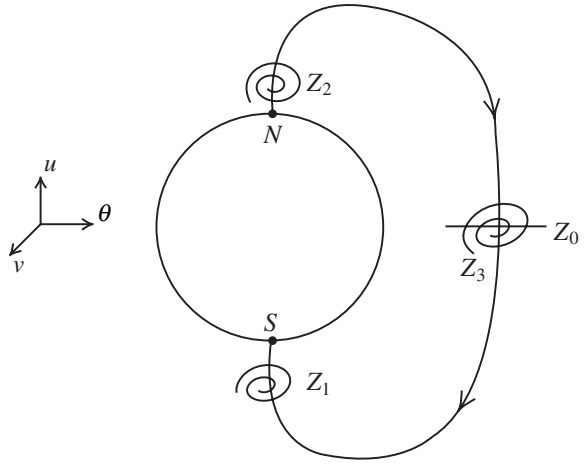

Figure 6. The path followed by the segment Z_0 along the flow of system (9) until it intersects itself (represented as Z_3) at at least a finite number of points.

s_2, close but beyond the collision of the homothetic orbit. Since equations (8) are continuous with respect to the initial data, the qualitative properties of segment L_1 are preserved by L_2.

The segment L_2 of (8) corresponds to a segment Z_2 of (9) at time τ_2. Z_2 lies very close to the north pole N, and since L_2 preserves the properties of L_1, Z_2 has at least a finite twist, which is further preserved when Z_2 travels along the flow of system (9) until it reaches the shape Z_3 at time τ_3. The twisted segment Z_3 has at least a finite intersection with the straight segment Z_0. This means that at least a finite number of solutions reach the zero-velocity curve at two different points. This implies that every negative energy level contains at least a finite number of symmetric periodic orbits.

Moreover, the above itinerary of Z_0 can be taken by the segment Z_3, which after passing beyond the collision manifold via system (8) intersects Z_0 again at least at a finite number of points. And we can repeat the procedure again a finite number of times. This completes the proof. □

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References

[D] Devaney R 1981 Singularities in classical mechanical systems *Ergodic Theory and Dynamical Systems I* (Boston: Birkhäuser) pp 211–333

[Di] Diacu F 1992 *Singularities of the N-Body Problem—An Introduction to Celestial Mechanics* (Montréal: Les Publications CRM)

[D-K] Diacu F, Kaplan S and Stoica C On the stability of the helium atom private communication

[D-M] Diacu F, Mioc V and Stoica C 2000 Phase-space structure and regularization of Manev-type problems *Nonlinear Anal.* **41** 1029–55

[L] Langmuir I 1921 The structure of the helium atom *Phys. Rev.* **17** 339–53

[LC] Levi-Civita T 1920 Sur la régularisation du probléme des trois corps *Acta Math.* **42** 99–144
[M] McGehee R 1974 Triple collision in the collinear three-body problem *Invent. Math.* **27** 191–227
[RT] Richter K, Tanner G and Wintgen D 1993 Classical mechanics of two-electron atoms *Phys. Rev.* A **48** 4182–96
[RW] Richter K and Wintgen D 1990 Analysis of classical motion on the Wannier ridge *J. Phys. B: At. Mol. Opt. Phys.* **23** L197–201
[TR] Tanner G, Richter K and Rost J M 2000 The theory of two-electron atoms: between ground state and complete fragmentation *Rev. Mod. Phys.* **72** 497–544