Braids with the symmetries of Platonic polyhedra in the Coulomb (N+1)-body problem

Marco Fenucci^{*} À

Àngel Jorba[†]

4 November 2019

Abstract

We take into account the Coulomb (N + 1)-body problem with N = 12, 24, 60. One of the particles has positive charge Q > 0, and the remaining N have all the same negative charge q < 0. These particles move under the Coulomb force, and the positive charge is assumed to be at rest at the center of mass. Imposing a symmetry constraint, given by the symmetry group of the Platonic polyhedra, we were able to compute periodic orbits, using a shooting method and continuation with respect to the value Q of the positive charge.

In the setting of the classical *N*-body problem, the existence of such orbits is proved with Calculus of Variation techniques, by minimizing the action functional. Here this approach does not seem to work, and numerical computations show that the orbits we compute are not minimizers of the action.

AMS Subject Classification: 70-08, 70F10, 34C25, 37N20, 65L07 Keywords: Coulomb potential, N-body problem, periodic solutions, choreographies

1 Introduction

The classical Newtonian N-body problem, for its history and its challenges, is a fundamental problem in mathematical physics. During the centuries, many mathematicians faced it, starting with Newton, who formulated the law of universal gravitation and solved the problem of two bodies, passing from Lagrange, who was the first to discover the triangular solutions of the three-body problem, through Poincaré which discovered the chaotic nature of the problem. In more recent years, the discovery of the Figure Eight solution of the three-body problem [20] started a research on particular periodic orbits of the N-body problem, that now are known with the name of *choreographies*. Numerical evidence of the existence of such orbits are given in [25–27], and also rigorous computer assisted methods to study their existence of the Figure Eight orbit was given in [5], and it uses the method of minimization of the action over a particular set of periodic loops. Since then, this technique has been used to prove the existence of other several periodic motions, see [2–6, 11–13, 19, 28, 29] and references therein. The idea of minimizing the action goes back to Poincaré [22].

Connection between the macroscopic scale, i.e. celestial mechanics, and the microscopic scale, i.e. the atomic mechanics, is given by the Coulomb force, which governs the interaction between

^{*}Dipartimento di Matematica, Università di Pisa, Largo B. Pontecorvo 5, 56127 Pisa, Italy

[†]Departament de Matemàtiques i Informàtica, Barcelona Graduate School of Mathematics (BGSMath), Universitat de Barcelona (UB), Gran Via de les Corts Catalanes 585, 08007 Barcelona, Spain

charged particles. The Coulomb potential depends on 1/r, as the Newtonian potential, with the difference that it depends on the charges and not on the masses. However, charges can be also negative, making this force both attractive and repulsive. The most famous connection is given by the Rutherford model of the atom [23], which represents the atom as a miniature Solar System. Since the introduction of quantum mechanics, this model was deprecated. However, despite quantum mechanics provides a more accurate description of nature, classical methods are still useful in studying atomic dynamics [30]. In more recent years, the Coulomb N-body problem, i.e. the problem of N charged particles which interact through the Coulomb force, was taken into account, and periodic orbits in the Coulomb three-body problem were found, see for example [14, 21, 24], trying to reproduce some features of the known orbits in the classical Newtonian three-body problem. On the other hand, some special symmetric solutions were found numerically in [7], for small values of N. The use of the Coulomb force as the only interacting force is motivated by the fact that the gravitational interaction is negligible when the electrostatic force is introduced in the system. Moreover, the Coulomb force by itself amounts to a non-relativistic approximation, which is reliable only when the velocities are small compared to the speed of light [18].

In this paper we consider the Coulomb (N+1)-body problem, composed by a positive charged particle and other N negative equally charged particles. We search for periodic motions sharing the symmetry of Platonic polyhedra, that is *Tetrahedron, Cube, Octahedron, Dodecahedron* and *Icosahedron*, hence N can be either 12, 24 or 60. For the Newtonian N-body problem, a list of orbits with this symmetry was found in [11]. Here we have been able to compute a similar set of periodic orbits, see the webpage [9] for animations of these solutions. Our numerical computations also show that these orbits are unstable. Moreover, since the approach used in [11,13] for the proof of the existence was the minimization of the action, here we investigated also if this method could still work for the Coulomb (N + 1)-body problem. However, we show numerically that the orbits we compute are not minimizers of the action, not even locally.

The paper is organized as follows. Section 2 introduces the model used. In Section 3 we describe the numerical methods used for the computation and in Section 4 we present the results obtained.

2 The Coulomb (N+1)-body problem

We take into account a system composed by N + 1 charged particles, one of which has positive charge and the rest have equal negative charges. Despite the Rutherford model [23] turned out to be not valid to represent the physical nature of the atom, for the sake of simplicity we will use terms as *electrons* and *nucleus* in the following.

We denote with q < 0, m > 0 the charge and the mass of the electron respectively, with Q > 0the charge of the nucleus, with $u_i \in \mathbb{R}^3, i = 1, ..., N$ the position of the *i*-th particle and with $u_0 \in \mathbb{R}^3$ the position of the nucleus. The mass of the nucleus is very high compared with the mass of the electrons, so we assume that the nucleus stays fixed at $u_0 \in \mathbb{R}^3$. The particles move under the Coulomb force, and the system of equations that determine the motion is given by

$$m\ddot{u}_{i} = \kappa q \bigg[\sum_{\substack{j=1\\j\neq i}}^{N} q \frac{u_{i} - u_{j}}{|u_{i} - u_{j}|^{3}} + Q \frac{u_{i} - u_{0}}{|u_{i} - u_{0}|^{3}} \bigg], \quad i = 1, \dots, N,$$
(1)

where $\kappa > 0$ is the Coulomb constant.

We choose a reference frame centered at the center of mass, hence from now on we assume

that $u_0 \equiv 0$. The system (1) is Lagrangian, and the Lagrangian L is given by

$$L = K + U,$$

where

$$K = \frac{1}{2} \sum_{i=1}^{N} m |\dot{u}_i|^2,$$
(2)

is the kinetic energy and

$$U = -\kappa \sum_{1 \le i < j \le N} \frac{q^2}{|u_i - u_j|} - \kappa \sum_{i=1}^N \frac{qQ}{|u_i|},$$
(3)

is the Coulomb potential. To simplify the computations, we can choose the units of charge, mass and distance so that

- the charge of the electron is unitary, hence q = -1,
- the mass of the electron is unitary, hence m = 1,
- the Coulomb constant is unitary, hence $\kappa = 1$.

Solutions to the equations (1) can be found also as stationary points of the Lagrangian action functional, defined as

$$\mathcal{A}(u) = \int_{a}^{b} L(u, \dot{u}) \, dt. \tag{4}$$

The functional (4) is defined over a set of curves $\mathcal{K} \subseteq H^1([a, b], \mathbb{R}^{3N})$, which has to be specified, depending on the problem that one wants to study.

2.1 Symmetry of the Platonic polyhedra and topological constraints

We want to compute periodic orbits of the system (1), imposing both symmetrical and topological constraints. As done in [11, 13], we take into account a Platonic polyhedron (i.e. *Tetrahedron*, *Cube*, *Octahedron*, *Dodecahedron* and *Icosahedron*) and we denote with \mathcal{R} its rotation group. We consider a system composed by $N = |\mathcal{R}|$ electrons (hence N can be either 12, 24 or 60) and, identifying $\{1, \dots, N\}$ with the elements of \mathcal{R} , we label the positions of the particles with the rotations of the group. We search for periodic orbits of period T > 0 such that

(a) the motion u_R , $R \in \mathcal{R} \setminus \{I\}$ is recovered by

$$u_R(t) = Ru_I(t), \quad t \in \mathbb{R};$$

(b) the trajectory of u_I , that we call generating particle, belongs to a given non-trivial freehomotopy class of $\mathbb{R}^3 \setminus \Gamma$, where

$$\Gamma = \bigcup_{R \in \mathcal{R} \setminus \{I\}} r(R),$$

and r(R) is the axis of the rotation R. Note that, by condition (a), $\Gamma \setminus \{0\}$ corresponds to the set of the partial collisions between the electrons;

(c) there exist $R \in \mathcal{R}$ and M > 0 such that

$$u_I(t+T/M) = Ru_I(t), \quad t \in \mathbb{R}.$$

In [11,13] periodic orbits of the N-body problem with equal masses, satisfying these symmetries and topological constraints, were found as minimizers of the Lagrangian action functional, using Calculus of Variations techniques in order to prove their existence.

In our case, taking into account the symmetry (a), the action functional writes as

$$\mathcal{A}(u) = N \int_0^T \left(\frac{1}{2} |\dot{u}_I|^2 - \frac{1}{2} \sum_{R \in \mathcal{R} \setminus \{I\}} \frac{1}{|(R-I)u_I|} + \frac{Q}{|u_I|}\right) dt,\tag{5}$$

and it is defined on the set

$$\mathcal{K} = \{ u \in H^1_T(\mathbb{R}, \mathbb{R}^{3N}) : \text{ (a), (b) and (c) hold} \}, \tag{6}$$

where $H_T^1(\mathbb{R}, \mathbb{R}^{3N})$ is the space of *T*-periodic loops of $H^1(\mathbb{R}, \mathbb{R}^{3N})$. Since a term with a negative sign appears in the Lagrangian, it is not clear whether this functional is coercive or not, and the search for periodic orbits using the usual minimization of the action technique does not apply so easily. For this reason we investigate the existence of these periodic orbits with a preliminary numerical study.

Note that (5) depends only on the path of the generating particle u_I . This means that we can reduce the searching for periodic orbits of the full system of charges to the searching of periodic orbits of the generating particle u_I , whose dynamics is defined by the Lagrangian

$$L = \frac{1}{2} |\dot{u}_I|^2 - \frac{1}{2} \sum_{R \in \mathcal{R} \setminus \{I\}} \frac{1}{|(R-I)u_I|} + \frac{Q}{|u_I|}.$$
(7)

The Euler-Lagrange equations of (7), written as first order system, are

$$\begin{cases} \dot{u}_{I} = v_{I}, \\ \dot{v}_{I} = \sum_{R \in \mathcal{R} \setminus \{I\}} \frac{(I - R)u_{I}}{|(R - I)u_{I}|^{3}} - \frac{Qu_{I}}{|u_{I}|^{3}}. \end{cases}$$
(8)

This system has the advantage that the dimension is much smaller than the dimension of the system of equations (1), 6 compared to 6N. Moreover, if the periodic orbit of the generating particle u_I is unstable in the system (8), then the complete orbit with N electrons is unstable in the system (1). On the other hand, the stability in the reduced system leads only to the stability with respect to symmetric perturbations of the complete orbit. To study entirely the stability, we need to solve equations (1), together with its variational equation, in order to compute the full $6N \times 6N$ monodromy matrix. Since we do not expect to find many stable orbits for the reduced system, the study of the stability is divided in two steps: at the first step we check whether the generating particle is stable in the reduced system or not and, if it is stable, we proceed in the computation of the full monodromy matrix and get an estimation the Floquet multipliers.

3 Numerical methods

In this section we describe the methods used to compute periodic orbits of (1) with the constraints described in Section 2. The main method is a variant of the well-known shooting method, but here

problems arise when we search for a good starting guess. In [11] the starting guess was computed using a gradient descent method, applied to the discretized version of the action functional of the N-body problem. In our case we cannot use the same method, because the lack of coercivity of the action (5) leads to a failure of the gradient method, that we experienced in our numerical experiments. A good starting guess is found applying a continuation method to a modification of the initial problem.

3.1 Shooting method

In order to compute the orbits, we use a shooting method in the phase space of the generating particle. The goal is to solve the boundary value problem

$$\begin{cases} \dot{x} = f(x), \\ x(T/M) = Sx(0), \end{cases}$$
(9)

where f is the vector field in (8), $x \in \mathbb{R}^6$, S is the matrix

$$S = \begin{pmatrix} R & 0 \\ 0 & R \end{pmatrix}$$

and $R \in \mathcal{R}$, M > 0 are given by condition (c) in Section 2.1. Fixed *n* values $0 = \tau_0 < \tau_1 < \cdots < \tau_n = T/M$, we define the function $G : \mathbb{R}^{6n} \to \mathbb{R}^{6n}$ as

$$\begin{cases} G_i = \phi^{\tau_i - \tau_{i-1}}(x_{i-1}) - x_i, & i = 1, \dots, n-1 \\ G_n = \phi^{\tau_n - \tau_{n-1}}(x_{n-1}) - Sx_0. \end{cases}$$
(10)

If we have a T-periodic solution x(t) satisfying (9), the function G evaluated at

$$X = (x(\tau_0), \ldots, x(\tau_{n-1}))$$

vanishes. Zeros of the function (10) are thus computed with a Newton method. The Jacobian matrix of G is

$$\frac{\partial G}{\partial X} = \begin{bmatrix} M_1 & -\operatorname{Id} & & \\ & M_2 & \ddots & \\ & & \ddots & -\operatorname{Id} \\ -S & & M_n \end{bmatrix},$$
(11)

where

$$M_i = \frac{\partial}{\partial x} \phi^{\tau_i - \tau_{i-1}}(x_i).$$

If X' denotes the new value of X at some iteration of the Newton method and $\Delta X = X' - X$, at each step we solve the linear system

$$\frac{\partial G}{\partial X}(X)\Delta X = -G(X). \tag{12}$$

However, the Jacobian matrix is singular at zeros of G, since we are free to choose the initial point along the periodic orbit. This degeneracy can be avoided as in [1], by adding a transversality condition on the first shooting point

$$f(x_0) \cdot \Delta x_0 = 0, \tag{13}$$

to the system (12), where $x_0, \Delta x_0$ are the first components of $X, \Delta X$ respectively. The system of equations (12), (13) has 6n + 1 equations and 6n unknowns, and we can solve it through the SVD decomposition, thus obtaining the value of ΔX .

Moreover, in order to make the method more stable, we choose to use a damped Newton method, i.e. the new value X' at the generic iteration is obtained as

$$X' = X + \gamma \Delta X. \tag{14}$$

The damping parameter γ is adaptive, since it is computed as

$$\gamma = \frac{\gamma_{\min}}{\max\left(\gamma_{\min}, \, |\Delta X|_{\infty}\right)},$$

where $|\Delta X|_{\infty} = \max_i |\Delta X_i|$. In our software we set $\gamma_{\min} = \frac{1}{10}$.

3.2 Continuation method

Suppose now that the vector field in (9) also depends on a real parameter, say λ , hence $f = f(x, \lambda)$. In this manner, the function G in (10) also depends on λ , hence $G = G(X, \lambda)$. As we will use the continuation method for different purposes, we explain it using a generic continuation parameter $\lambda \in \mathbb{R}$. Given a couple $(X_i, \lambda_i)^T$ such that $G(X_i, \lambda_i) = 0$, we want to continue this solution with respect to the varying parameter λ , in order to find a curve of solutions parametrized with λ . To this end, we add to the system (10) an equation to displace the entire couple $(X, \lambda)^T$. The system we solve is therefore

$$\begin{cases} G(X,\lambda) = 0, \\ \left| \begin{pmatrix} X_i \\ \lambda_i \end{pmatrix} - \begin{pmatrix} X \\ \lambda \end{pmatrix} \right|^2 - \delta^2 = 0, \end{cases}$$
(15)

where, as usual, $|\cdot|$ denotes the Euclidean norm and $\delta > 0$ is a positive parameter determining the displacement along the curve of solutions. The solution $(X_{i+1}, \lambda_{i+1})^T$ of system (15) is computed using again a Newton method, solving at each step a linear system given by the matrix

$$\begin{bmatrix} \frac{\partial G}{\partial X} & \frac{\partial G}{\partial \lambda} \\ 2(X - X_i) & 2(\lambda - \lambda_i) \end{bmatrix}.$$
 (16)

The initial guess can be constructed starting from the known solution $(X_i, \lambda_i)^T$, and taking a tangent displacement along the curve of solutions. However, we have simply constructed the initial guess by approximating this tangent line using two previous different solutions, say $(X_i, \lambda_i)^T$ and $(X_{i-1}, \lambda_{i-1})^T$, as

$$\begin{pmatrix} \hat{X} \\ \hat{\lambda} \end{pmatrix} = \begin{pmatrix} X_i \\ \lambda_i \end{pmatrix} + \gamma \begin{pmatrix} X_i - X_{i-1} \\ \lambda_i - \lambda_{i-1} \end{pmatrix}, \qquad \gamma = \frac{\delta}{|(X_i, \lambda_i)^T - (X_{i-1}, \lambda_{i-1})^T|}.$$

As we are searching for periodic solutions, for the reasons explained above, we have added the transversality condition (13). The final system we have to solve at each step is non-squared, and we use again the SVD decomposition to solve it.

Note also that, since G is defined through the flow of an ordinary differential equation and we need to compute the derivatives of G with respect to the parameter λ , we have to compute the derivatives of the flow with respect to λ . To do this, the system of equations that we have to solve numerically is

$$\begin{cases} \dot{x} = f(x,\lambda), \\ \dot{A} = \frac{\partial f(x,\lambda)}{\partial x} A, \\ \dot{w} = \frac{\partial f(x,\lambda)}{\partial x} w + \frac{\partial f(x,\lambda)}{\partial \lambda}, \end{cases}$$
(17)

where $x, w \in \mathbb{R}^6, A \in \mathbb{R}^{6 \times 6}$ and $\lambda \in \mathbb{R}$. Indeed, the second equation gives the derivatives of the flow ϕ^t with respect to the initial condition x, while the third equation gives the derivatives of the flow ϕ^t with respect to the parameter λ .

3.3 Computing periodic orbits

As it has been mentioned before, one of the difficulties to carry out these computations is to find a good initial guess for the Newton method to converge. To deal with this, we have used two different continuation schemes.

From the physical intuition, if the central charge is zero, the electrons only repel each other, and we do not expect to find any periodic solutions. For continuity reasons, if the central charge is too small compared to the number of electrons, a periodic orbit could still not exist. On the contrary, if the positive charge is large enough, the contribution of the electrons in the vector field (1) is small, compared to the term given by the positive charge. Indeed, rescaling the loops as $u_i(t) = Q^{1/3}v_i(t)$, $i = 1, \ldots, N$ in (1), we obtain a differential equation for v_i , which writes as

$$\ddot{v}_i = \mu \sum_{\substack{j=1\\j\neq i}}^N \frac{v_i - v_j}{|v_i - v_j|^3} - \frac{v_i}{|v_i|^3}, \quad i = 1, \cdots, N,$$

where $\mu = Q^{-1/3}$. Note that, when the positive charge is ideally "infinite", the interactions between the different electrons disappear, and the differential equation that determines the motion of v_i is the equation of a Kepler problem. Intuitively, when the central charge is finite but very large, the solution is close to a circular piecewise loop, composed by Keplerian arcs, joined at points on the collision lines. Therefore, physical intuition suggests that periodic solutions are more likely to exist when the central charge is large enough. For all these reasons it is easier to find periodic orbits for high values of the central charge and to continue them to lower values of Q.

To find periodic orbits for large values of Q we use the following strategy. First we choose a closed curve

$$\varphi: [0,T] \to \mathbb{R}^6, \qquad \varphi(t) = \left(u(t), \dot{u}(t)\right)^T,$$

such that the image of the spatial component u([0,T]) belongs to the chosen free-homotopy class of $\mathbb{R}^3 \setminus \Gamma$. Moreover, we can take this spatial component to be on a sphere, since we expect that the final orbit does not have large changes in the radial component. Of course this curve will not solve equation (9), but we can perturb the system and define a new differential equation for which φ is a solution. Indeed, if we define

$$\dot{x} = f(x) - \varepsilon \psi(t), \tag{18}$$

where

$$\psi(t) = \dot{\varphi}(t) - f(\varphi(t)),$$

then $\varphi(t)$ is a solution of (18) for $\varepsilon = 1$. To find the periodic orbit for $\varepsilon = 0$, we consider ε as a parameter and we use the continuation method. In our computations, we decided to stop the continuation when we reach a value of $\varepsilon < 10^{-2}$: this was usually enough to have an initial guess for the shooting method to converge for $\varepsilon = 0$ and compute the periodic orbits.

Summarizing, the approach used to compute the orbits is the divided in three steps.

- Step 1: We generate a starting guess for a high value of the central charge Q, with the method described above. In our computations, we decided to choose a value near 2N, i.e. two times the number of electrons.
- Step 2: We compute the solution using the shooting method described in Section 3.1, with the same value of Q used to produce the initial guess, and using continuation w.r.t. ε as explained above, until we reach $\varepsilon = 0$. Using this last solution as starting guess, we compute a second solution for the value of the central charge equal to Q 1: this is needed to start the continuation w.r.t. the value of the central charge.
- Step 3: Using the two solutions computed at the Step 2, we start the continuation method described in Section 3.2, in order to find solutions for smaller values of Q.

4 Results of the computations

In [11], for each Platonic polyhedron, a list of free-homotopy classes of $\mathbb{R}^3 \setminus \Gamma$, each one containing a collision-free minimizer of the N-body problem with equal masses, were provided: these lists are available at [10]. Here we search for symmetric periodic solutions of the system (1), in the same free-homotopy classes listed at [10]. In [11], 9 and 57 homotopically different periodic orbits with the symmetry of the Tetrahedron and the Cube, respectively, were found for the N-body problem with equal masses. The total number of orbits with the symmetry of the Dodecahedron was 1442, but the entire computation of all of them was not done. Here we were able to compute all these orbits also in Coulomb (N + 1)-body problem introduced in Section 2, with the symmetry of the Tetrahedron and the Cube, reproducing the list in [10]. For the symmetry of the Dodecahedron only a few number of orbits were computed (a large number of them is expected). Examples of orbits with 24 electrons are displayed in Figure 1. More images and videos are available at the webpage [9].

4.1 Continuation

In our computations we set the period to be T = 1: this is not restricting, since an orbit with an arbitrary period can be found simply by rescaling size and time. During the continuation process we always reached a turning point in Q. This means that, when we were able to reach the physical situation of negative charged ions (i.e. when Q < N), we can continue the solutions following the turning point, and find a second orbit in which the system is neutral (i.e. when Q = N). This does not happen in all the cases we tried, and it is not clear if there is an additional topological condition to be satisfied in order to have the turning point below Q = N.

4.2 Stability

As said before, the study of the stability is divided in two steps: first we study the stability of the orbit of the generating particle in the reduced system (7), computing a 6×6 monodromy matrix M_6 . If the generating particle in unstable, then also the complete orbit in the system (1) is unstable, otherwise we proceed in the computation of the complete $6N \times 6N$ monodromy matrix

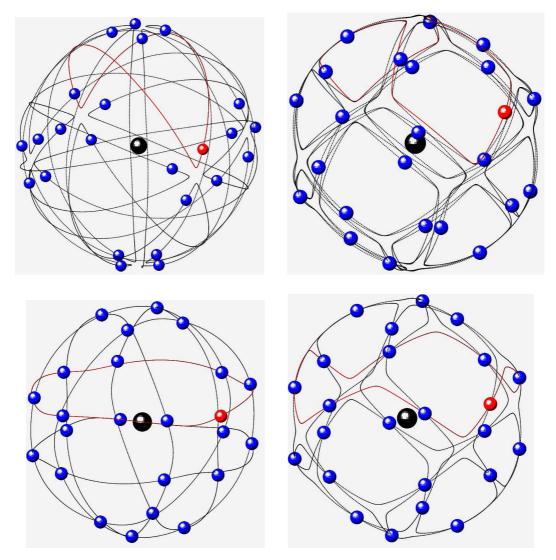


Figure 1: Solutions with 24 electrons and the symmetry of the Cube. The value of the central charge is 24 for all the four examples. The homotopy class for the orbits on top is ν_2 and ν_{43} for the orbits on bottom. The enumeration is referred to the website [9]. The red electrons represent the generating particles, and the red curve are their trajectories. The black particle in the middle is the nucleus. The orbits on the right are obtained by the continuation method, starting from the orbits on the left. We reached them after following a turning point on the curve of solutions.

 M_{6N} . During the continuation, the six eigenvalues of M_6 move in the complex plane. For the most of the orbits, looking at the eigenvalues of M_6 was enough to conclude the instability, since during the continuation a very large Floquet multiplier (of the order that ranges from 10^6 to 10^{20} , depending on the orbit) appears. However, it can happen that for certain values of the central charge, the eigenvalues of M_6 are all on the unit circle, meaning that the generating particle is stable in the reduced system. In these few cases we computed the matrix M_{6N} , verifying that the complete orbit is indeed unstable, since a large Floquet multiplier arises. An example of this situation is reported in Figure 2. More figures of this kind can be found at [9]. From the computations, it results that all the orbits are unstable. Results for the orbits with the symmetry of the Tetrahedron are summarised in Table 1.

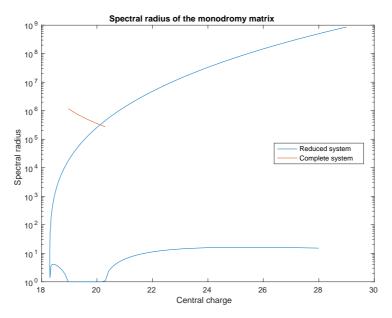


Figure 2: The spectral radius of the monodromy matrix. On the x axis is reported the value of the central charge and on the y axis is reported the value of the spectral radius, in logarithmic scale. The blue curve represent the evolution of the spectral radius of the monodromy matrix in the reduced system, while the red curve represent the evolution of the spectral radius in the complete system. During the continuation, the generating particle becomes stable for certain values of Q (near Q = 20, blue curve), but in fact the resulting complete orbit is unstable (red curve). This plot is referred to the orbits in Figure 1, bottom.

4.3 Are these orbits minimizers?

To understand better the variational nature of the orbits computed, we wonder whether they are minimizers of the action (5) or not. Verify that the orbits are global minimizers is hard to do with only numerical methods, since all the loops have to be taken into account. However, we can verify if they are at least directional local minimizers, weak local minimizers or strong local minimizers. To this end, we recall here briefly the definitions and the results that we need.

Formulation of the problem Fixed T > 0, let us consider a functional

$$\mathcal{A}(u) = \int_0^T L(t, u, \dot{u}) dt, \tag{19}$$

where $L: [0,T] \times \Omega \to \mathbb{R}$ is a C^2 function, *T*-periodic in the variable *t*, and $\Omega \subseteq \mathbb{R}^n \times \mathbb{R}^n$ is an open set. We define the space of the *T*-periodic functions

$$V = \{ u \in C^1([0,T], \mathbb{R}^n) : u(0) = u(T) \}.$$

and we consider \mathcal{A} defined on a subset $X \subseteq V$.

Definition 1. We say that $u_0 \in X$ is a

(GM) global minimum point if $\mathcal{A}(u) \geq \mathcal{A}(u_0)$ for all $u \in X$;

(SLM) strong local minimum point if there exists $\varepsilon > 0$ such that for all $u \in X$ satisfying

$$\|u-u_0\|_{\infty} < \varepsilon;$$

we have that $\mathcal{A}(u) \geq \mathcal{A}(u_0)$;

label	$\min Q$	$\left \lambda\right \left(Q=\min Q\right)$	$\left \lambda_{6N}\right \left(Q=\min Q\right)$	$\left \lambda\right \left(Q=12\right)$
ν_1	10.346970805	7.3761606	/	$0.18050567 \cdot 10^4$
$ u_2 $	8.2812509283	2.5911113	/	$0.26940597\cdot 10^4$
ν_3	9.9652582174	3.7293607	/	$0.49658024 \cdot 10^2$
ν_4	12.905694682	1.0	$0.4930569 \cdot 10^5$	/
ν_5	8.7205631222	$0.28289539 \cdot 10^3$	/	$0.33578812 \cdot 10^9$
$ u_6 $	9.5460053624	$0.49445974\cdot 10^2$	/	$0.27073516 \cdot 10^5$
ν_7	8.0760877496	$0.18090607 \cdot 10^5$	/	$0.33898930 \cdot 10^{13}$
ν_8	12.905977225	2.8508903	/	/
$ u_9$	12.905656346	1.0	$0.2461446\cdot 10^{10}$	/

Table 1: Some numerical values obtained for the orbits with the symmetry of the Tetrahedron. Second column contains an approximation of the minimal value of the central charge Q obtained during the continuation. Third column contains the spectral radius of the monodromy matrix M_6 for $Q = \min Q$. When this value is equal to 1, we report the spectral radius of the complete monodromy matrix M_{6N} in column four. Last column contains the value of the spectral radius of M_6 for Q = 12, for which the system is neutral. The labels correspond to the enumeration used in the website [9].

(WLM) weak local minimum point if there exists $\varepsilon > 0$ such that for all $u \in X$ satisfying

$$\left\|u-u_{0}\right\|_{\infty}+\left\|\dot{u}-\dot{u}_{0}\right\|_{\infty}<\varepsilon;$$

we have that $\mathcal{A}(u) \geq \mathcal{A}(u_0)$;

(DLM) directional local minimum point (DLM) if the function

$$\varphi(s) := \mathcal{A}(u_0 + sv),$$

has a local minimum point at s = 0 for all $v \in V$. Note that, fixed $v \in V$, $\varphi : (-\delta, \delta) \to \mathbb{R}$ is a function of the real variable s.

It is clear that (GM) implies (SLM), which implies (WLM), which implies (DLM). Moreover, it is known that a necessary condition for a regular function u_0 to be a (DLM) is that it solves the Euler-Lagrange equation associated to (19), i.e.

$$\frac{d}{dt}L_{\dot{u}}(t, u_0(t), \dot{u}_0(t)) = L_u(t, u_0(t), \dot{u}_0(t))$$
(20)

Note also that a solution u_0 of (20) is a (DLM) if and only if the second variation

$$\delta^2 \mathcal{A}(v) = \int_0^T \left(v(t) \cdot \hat{L}_{uu}(t) v(t) + 2\dot{v}(t) \cdot \hat{L}_{u\dot{u}}(t) v(t) + \dot{v}(t) \cdot \hat{L}_{\dot{u}\dot{u}}(t) \dot{v}(t) \right) dt,$$

is non-negative for all $v \in V$, where

$$\begin{split} \hat{L}_{uu}(t) &= L_{uu}(t, u_0(t), \dot{u}_0(t)), \\ \hat{L}_{u\dot{u}}(t) &= L_{u\dot{u}}(t, u_0(t), \dot{u}_0(t)), \\ \hat{L}_{\dot{u}\dot{u}}(t) &= L_{\dot{u}\dot{u}}(t, u_0(t), \dot{u}_0(t)). \end{split}$$

The second variation is a *quadratic functional*. Necessary and sufficient conditions for a quadratic functional to be positive definite are given in [8], for general boundary conditions. We recall briefly here the main theorem and the definitions needed to state it.

Quadratic functionals Let $[a, b] \subseteq \mathbb{R}$ be a closed interval, we consider a general quadratic functional

$$\mathcal{Q}(v) = \int_{a}^{b} \left(v \cdot P(t)v + 2\dot{v} \cdot Q(t)v + \dot{v} \cdot R(t)\dot{v} \right) dt,$$
(21)

where $P, Q, R : [0,T] \to \mathbb{R}^{n \times n}$ are C^1 matrix functions such that $P(t) = P^T(t), R(t) = R^T(t)$ for all $t \in [0,T]$. Given a matrix $D \in \mathbb{R}^{2n \times 2n}$, we consider \mathcal{Q} defined on functions $v : [a,b] \to \mathbb{R}^n$ such that

$$D\begin{pmatrix}v(a)\\v(b)\end{pmatrix} = 0.$$
(22)

The Euler-Lagrange equation associated to (21) is

$$\frac{d}{dt}[R\dot{y} + Qy] = Q^T\dot{y} + Py,$$

and it is usually called *Jacobi differential equation*. If det $R(t) \neq 0$ for all $t \in [0, T]$, we can write the system as

$$\begin{cases} \dot{y} = Ay + Bz, \\ \dot{z} = Cy - A^T z, \end{cases}$$
(23)

where

$$A = -R^{-1}Q, \quad B = R^{-1}, \quad C = P - Q^T R^{-1}Q.$$

Note that B, C are symmetric matrices. It is useful to define also the matrix version of the equation, i.e.

$$\begin{cases} \dot{Y} = AY + BZ, \\ \dot{Z} = CY - A^T Z, \end{cases}$$
(24)

where $Y, Z : [0, T] \to \mathbb{R}^{n \times n}$ are matrix functions. We introduce now some conditions and give some definitions, useful to state the main theorem.

Definition 2. Let (y, z) be a solution of system (23) such that y(a) = 0. A point $c \in (a, b]$ is said to be *conjugate* with a if

$$y(c) = 0.$$

Definition 3. We say that the strengthened Legendre condition (L') holds if $R(t) > 0^{-1}$ for all $t \in [a, b]$ for all $t \in [a, b]$.

Definition 4. We say that the strengthened Jacobi condition (J') holds if every solution (y, z) of (23) with initial condition y(a) = 0 does not have any conjugate point $c \in (a, b]$ with a.

Note that condition (J') is equivalent in saying that the solution (Y_a, Z_a) of (24) with initial conditions

$$\begin{cases} Y_a(a) = 0, \\ Z_a(a) = \mathrm{Id}, \end{cases}$$

is such that det $Y_a(t) \neq 0$ for $t \in (a, b]$. The following theorem gives necessary and sufficient conditions for Q to be positive definite.

¹In the following, when we write A > 0 $(A \ge 0)$, where $A \in \mathbb{R}^{n \times n}$ is a symmetric matrix, we mean that A is positive definite (positive semi-definite).

Theorem 1. Let condition (L') hold. We have that

$$\mathcal{Q}(v) > 0,$$

for any nonzero v satisfying (22) if and only if condition (J') holds and

$$\alpha^{T} \begin{pmatrix} -W_{b}(a) & -Y_{a}^{-1}(b) \\ -Y_{a}^{T-1}(b) & W_{a}(b) \end{pmatrix} \alpha > 0$$

$$(25)$$

for all nonzero $\alpha \in \mathbb{R}^{2n}$ such that $D\alpha = 0$. Here (Y_a, Z_a) , (Y_b, Z_b) are the solutions of (24) given by the initial conditions

$$\begin{cases} Y_a(a) = 0, \\ Z_a(a) = \mathrm{Id}, \end{cases} \qquad \begin{cases} Y_b(b) = 0, \\ Z_b(b) = -\mathrm{Id}, \end{cases}$$

and $W_a = Z_a Y_a^{-1}, W_b = Z_b Y_b^{-1}.$

The case of symmetric orbits in the Coulomb (N+1)-body problem

We take into account the symmetry of the space of loops in the theory summarized above modifying the minimization problem. Let $u : [0,T] \to \mathbb{R}^{3N}$ be a loop satisfying condition (a) and the additional choreography constraint

$$u_I\left(t+\frac{T}{M}\right) = Ru_I(t), \quad t \in [0,T],$$

for a given $R \in SO(3)$ and $M \in \mathbb{N}$. For the sake of simplicity, we will work with the function u_I , which represents the motion of a single electron along the periodic orbit. From expression (5), we have that

$$\int_{0}^{T} L(u_{I}, \dot{u}_{I}) dt = M \int_{0}^{\frac{T}{M}} L(u_{I}, \dot{u}_{I}) dt.$$
(26)

We consider the functional

$$\bar{\mathcal{A}}(u_I) = \int_0^{T/M} \left(\frac{1}{2}|\dot{u}_I|^2 - \frac{1}{2}\sum_{R\in\mathcal{R}\setminus\{I\}} \frac{1}{|(R-I)u_I|} + \frac{Q}{|u_I|}\right) dt,$$

defined on the set of loops

$$u_I: \left[0, \frac{T}{M}\right] \longrightarrow \mathbb{R}^3,$$

such that $Ru_I(0) = u_I(T/M)$. Note that, by means of (26), if $u_I^* : [0,T] \to \mathbb{R}^3$ is a minimizer of the functional \mathcal{A} , then the restriction

$$u_I^*|_{[0,T/M]}: \left[0, \frac{T}{M}\right] \longrightarrow \mathbb{R}^3,$$

is a minimizer of $\overline{\mathcal{A}}$. Vice versa, if $u_I^* : [0, T/M] \to \mathbb{R}^3$ is a minimizer of $\overline{\mathcal{A}}$, then we can extend it to a closed loop $u_I^* : [0, T] \to \mathbb{R}^3$, simply by using the rotation R, and we obtain a minimizer for \mathcal{A} .

Therefore, for the functional \overline{A} , we have that [a, b] = [0, T/M]. Moreover, the matrix D defining the admissible curves for the second variation is

$$D = \begin{pmatrix} R & -\mathrm{Id} \\ 0 & 0 \end{pmatrix} \in \mathbb{R}^{6 \times 6}.$$

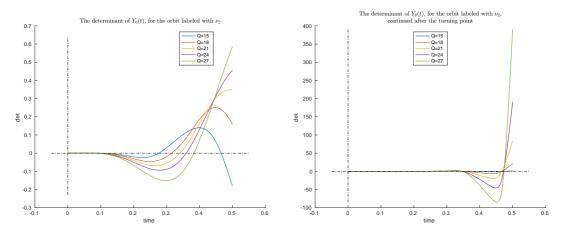


Figure 3: The determinant of the matrix $Y_0(t)$ in the fundamental interval [0, T/M] = [0, 1/2], for different values of the central charge Q. These plots are referred to the periodic orbits in Figure 1, top.

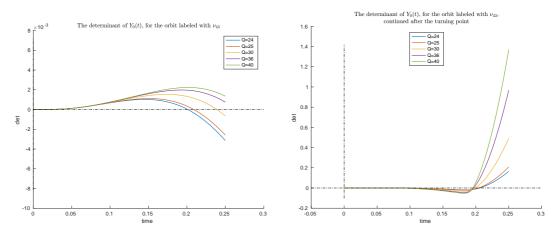


Figure 4: The determinant of the matrix $Y_0(t)$ in the fundamental interval [0, T/M] = [0, 1/2], for different values of the central charge Q. These plots are referred to the periodic orbits of Figure 1, bottom.

Therefore, a vector $\alpha \in \mathbb{R}^6$ satisfying $D\alpha = 0$ is of the form

$$\alpha = \begin{pmatrix} \beta \\ R\beta \end{pmatrix},$$

where $\beta \in \mathbb{R}^3$. Inserting this relation in (25), we obtain that the second variation associated to a solution of Euler-Lagrange equation u_0 is positive definite if and only if (J') holds and the 3×3 matrix

$$-W_{T/M}(0) - Y_0^{-1}(T/M)R - R^T Y_0^{T-1}(T/M) + R^T W_0(T/M)R$$
(27)

is positive definite. Note that condition (L') is always satisfied, since we have that

$$\frac{\partial^2 L}{\partial \dot{u}_I^2} = \mathrm{Id} \,.$$

To decide whether a solution that we compute is actually a local minimizer or not, we check if it is a (DLM) or not. To do so, we search for conjugate points in the fundamental interval [0, T/M], simply by computing the solution (Y_0, Z_0) of (24) with initial conditions

$$\begin{cases} Y_0(0) = 0, \\ Z_0(0) = \mathrm{Id}, \end{cases}$$

and then plotting the determinant of $Y_0(t)$. Since the computation is quite fast, we can also see how the determinant evolves with respect to the value of the central charge Q, including its computation in the continuation process. Most of the orbits computed have a behaviour similar to the one shown in Figure 3, i.e. they have at least a conjugate point in the fundamental interval [0, T/M], indicating that they are not minimizers, not even directional. Moreover, after the turning point the presence of a conjugate point seems to be more likely, also because we saw that the value of the action of the periodic orbit generically increase with respect to the previous orbit with the same value of Q.

However, it can occur that, during the continuation process, the determinant of $Y_0(t)$ does not vanish for certain values of the central charge Q. For example, in Figure 4, we can see that the determinant is positive for the values Q = 36, 40. Continue increasing the value of the charge Q, this behaviour still persists, and it seems that the determinant has a limiting curve that does not vanish in the fundamental interval (0, 1/4]. Hence we also have to compute the matrix in (27), and verify whether it is positive definite or not. In this case, the eigenvalues of the matrix in (27), for Q = 40, are computed to be

$$14.723038, 5.5236623, -307.98056,$$

hence this orbit is also not a local minimizer, despite the absence of conjugate points. For values of Q > 40, this property still holds, and the negative eigenvalue seems to converge to a value close to -60.757245.

Further computations for the remaining orbits show that the two described behaviours are common to all of them, suggesting that they are not local minimizers, but indeed different kind of stationary points, such as saddles. For this reason the method of minimization of the action does not seem to work for the Coulomb (N+1)-body problem to find periodic orbits, and maybe other variational techniques have to be used to provide a rigorous proof of their existence.

Acknowledgments

The first author acknowledges the project MIUR-PRIN 20178CJA2B titled "New frontiers of Celestial Mechanics: theory and applications". The second author has been supported by the Spanish grants PGC2018-100699-B-I00 (MCIU/AEI/ FEDER, UE) and the Catalan grant 2017 SGR 1374. The project leading to this application has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 734557.

References

- A. Abad, R. Barrio, and A. Dena. Computing periodic orbits with arbitrary precision. *Phys. Rev. E*, 84:016701, 2011.
- [2] K.-C. Chen. Binary decompositions for planar N-body problems and symmetric periodic solutions. Arch. Ration. Mech. Anal., 170(3):247–276, 2003.

- [3] K. C. Chen. Existence and minimizing properties of retrograde orbits to the three-body problem with various choices of masses. *Annals of Mathematics*, 167(2):325–348, 2008.
- [4] A. Chenciner. Action minimizing solutions of the newtonian n-body problem: from homology to symmetry. In Proceedings of the International Congress of Mathematicians, Vol. III (Beijing, 2002), pages 279–294. Higher Ed. Press, Beijing, 2002.
- [5] A. Chenciner and R. Montgomery. A remarkable periodic solution of the three-body problem in the case of equal masses. *Annals of Mathematics*, 152(3):881–901, 2000.
- [6] A. Chenciner and A. Venturelli. Minima de l'intégrale d'action du problème newtonien de 4 corps de masses égales dans R³: orbites "hip-hop". Cel. Mech. Dyn. Ast., 77(2):139–152, 2000.
- [7] I. Davies, A. Truman, and Z. Williams. Classical periodic solutions of the equal-mass 2nbody problem, 2n-ion problem and the n-electron atom problem. *Physics Letters A*, 99(1):15 - 18, 1983.
- [8] Z. Došlá and O. Došlý. Quadratic functionals with general boundary conditions. Appl. Math. Optim., 36(3):243-262, 1997.
- [9] M. Fenucci. http://adams.dm.unipi.it/~fenucci/research/coulomb.html.
- [10] M. Fenucci. http://adams.dm.unipi.it/~fenucci/research/nbody.html.
- [11] M. Fenucci and G. F. Gronchi. On the stability of periodic N-body motions with the symmetry of platonic polyhedra. *Nonlinearity*, 31(11):4935, 2018.
- [12] D. L. Ferrario and S. Terracini. On the existence of collisionless equivariant minimizers for the classical n-body problem. *Inventiones mathematicae*, 155(2):305–362, 2004.
- [13] G. Fusco, G. F. Gronchi, and P. Negrini. Platonic polyhedra, topological constraints and periodic solutions of the classical N-body problem. *Inventiones mathematicae*, 185(2):283–332, 2011.
- [14] M. Šindik, A. Sugita, M. Šuvakov, and V. Dmitrašinović. Periodic three-body orbits in the Coulomb potential. *Phys. Rev. E*, 98:060101, Dec 2018.
- [15] T. Kapela and C. Simó. Computer assisted proofs for nonsymmetric planar choreographies and for stability of the eight. *Nonlinearity*, 20:1241–1255, 2007.
- [16] T. Kapela and C. Simó. Rigorous KAM results around arbitrary periodic orbits for Hamiltonian systems. *Nonlinearity*, 30(3):965–986, 2017.
- [17] T. Kapela and P. Zgliczynski. The existence of simple choreographies for the N-body problem - a computer assisted proof. Nonlinearity, 16(6):1899–1918, 2003.
- [18] L. D. Landau and E. M. Lifshitz. The Classical Theory of Fields. Butterworth-Heinemann, 4 edition, 1980.
- [19] C. Marchal. How the method of minimization of action avoids singularities. Celestial Mech. Dynam. Astronom., 83(1-4):325–353, 2002. Modern celestial mechanics: from theory to applications (Rome, 2001).
- [20] C. Moore. Braids in classical dynamics. Phys. Rev. Lett., 70(24):3675–3679, 1993.

- [21] F. Pérez and J. Mahecha. Classical trajectories in Coulomb three body systems. Rev. Mexicana Fís., 42(6):1070–1086, 1996.
- [22] H. Poincaré. Sur les solutions périodiques et le principe de moindre action. C. R. Acad. Sci., 123:915–918, 1896.
- [23] E. Rutherford. The scattering of α and β particles by matter and the structure of the atom. *Philosophical Magazine*, 21(125):669–688, 1911.
- [24] A. Santander, J. Mahecha, and F. Pérez. Rigid-rotator and fixed-shape solutions to the Coulomb three-body problem. *Few-Body Systems*, 22(1):37–60, Feb 1997.
- [25] C. Simó. New families of solutions in N-body problems. In Carles Casacuberta, Rosa Maria Miró-Roig, Joan Verdera, and Sebastià Xambó-Descamps, editors, *European Congress* of Mathematics: Barcelona, July 10–14, 2000, Volume I, pages 101–115, Basel, 2001. Birkhäuser Basel.
- [26] C. Simó. Periodic orbits of the planar N-body problem with equal masses and all bodies on the same path, pages 265–284. IoP Publishing, 2001.
- [27] C. Simó. Dynamical properties of the figure eight solution of the three-body problem. In *Celestial mechanics (Evanston, IL, 1999)*, volume 292 of *Contemp. Math.*, pages 209–228. Amer. Math. Soc., Providence, RI, 2002.
- [28] S. Terracini. On the variational approach to the periodic *n*-body problem. Cel. Mech. Dyn. Ast., 95:3–25, 2006.
- [29] S. Terracini and A. Venturelli. Symmetric trajectories for the 2N-body problem with equal masses. Arch. Ration. Mech. Anal., 184(3):465–493, 2007.
- [30] T. Uzer, D. Farrelly, J. A. Milligan, P. E. Raines, and J. P. Skelton. Celestial mechanics on a microscopic scale. *Science*, 253(5015):42–48, 1991.