Coulomb Mechanics

(Project 2018-3 proposed by Malyshev V.A.)

0.1 Axioms

Besides Axiom-Newton we assume

Coulomb force (Axiom-Coulomb) Only forces defined by

$$U_{jk}(|x_k - x_j|) = \frac{q_k q_j}{|x_k - x_j|}$$

can be used, where $q_i \in R$ is the electric charge of particle i.

0.2 Main goals

The situation seems to be similar to that of the great science called Celestial Mechanics. However, I was greatly surprised when I could not find any mathematical paper on Coulomb mechanics concerning bounded trajectories. Possibly new types of such trajectories exist, then I will be grateful if someone will indicate the references.

The first goal is to study bound states for small $N \geq 3$. We call **bound state** the set of trajectories $x_i(t), i = 1, \dots, N$, of N particles such that for some constants $0 < C_1 < C_2$ and all i, j, t

$$C_1 < |x_i(t) - x_j(t)| < C_2$$

Example of bound state is a **fixed state**, that is the set $\{x_1, \dots, x_N\}$ of N points so that $x_i(t) \equiv x_i$ for all t and $i = 1, \dots, N$.

The central intuitive idea of Celestial Mechanics is that bound states exist due to equilibrium of Newton gravitation force and centrifugal force. Coulomb mechanics does not still exist but it is very likely that the bound states have much richer structure.

0.3 Easy cases

0.3.1 Complete repulsion

Problem (to prove) If the charges of all N particles $i = 1, 2, \dots, N$ have the same sign, then as $t \to \infty$ for any $i \neq j$ and any initial conditions

$$|x_i(t) - x_j(t)| \to \infty$$

as $t \to \infty$.

0.3.2 Two particles

If $N = 2$ and the particle charges have different signs, then there is complete coincidence with Celestial mechanics.

Existence of atoms in Coulomb Mechanics According to physics, we call atom in Coulomb mechanics the system consisting of one particle with positive charge ("nucleus") and $k \geq 1$ negative charge particles ("electrons") rotating around the "nucleus". We have mentioned above that existence for $k = 1$ is the first result of Celestial mechanics (Kepler orbit). The existence of atoms in Coulomb mechanics for $k > 1$ formally does not follow from Celestial Mechanics, because of mutual repulsion of electrons, but one could guess that it can be deduced similarly to Celestial mechanics, for example in some cases using perturbation theory.

0.3.3 Three particles in dimension 1

It is known that in dimension 3 there are no (due to harmonicity of the potential $\frac{1}{r}$) stable fixed configurations. However, stability problem in dimensions 1 and 2 can give some insight on other and more complicated problems in dimension 3. It is clear that for two particles there are no fixed configurations. But for 3 particles they exist already in dimension 1.

Two particles have infinite masses This means that two particles (1 and 2) have fixed trajectories and particle 3 moves in their Coulomb field. In particular, here we assume that particles 1 and 2 stand still. Already here new phenomena (compared to celestial mechanics) appear.

Thus, assume that on the real line R there are particles 1,2,3 with charges $q_1, q_2, q_3 = q$ and coordinates $x_1(t) \equiv 0, x_2(t) \equiv a, x_3(0) = x(0)$ correspondingly.

Case $\boldsymbol{0 < a < x(0)}$ We consider the following problem: for which parameters and initial conditions $x_3(0) = x(0), v_3(0) = v(0)$ we have $C_1 < x(t) < C_2$ for some $C_1 > a$ and $C_2 < \infty$, that is **bound states** exist.

Proposition 1. There is exactly one fixed state if either $0 < |q_2| < q_1, q_2 < 0$, (unstable fixed state) or $0 < q_2 < |q_1|, q_1 < 0$, (stable fixed state). Otherwise there are no fixed states.

Moreover, initial conditions define bound states only when $0 < q_2 < |q_1|, q_1 < 0$, and

$$H(0) = \frac{mv^2(0)}{2} + U(0) < 0$$

Proof. Particle 3 moves in the Coulomb fields of particles 1 and 2, that is in the potential field

$$U(x) = q\Big(\frac{q_1}{|x|} + \frac{q_2}{|x - x_2|}\Big) = q\Big(\frac{q_1}{x} + \frac{q_2}{x - x_2}\Big) = q\frac{(q_1 + q_2)x - x_2 q_1}{x(x - x_2)}, \quad (1)$$

or in the force field

$$F(x) = -\frac{\partial U}{\partial x} = q\Big(\frac{q_1}{x^2} + \frac{q_2}{(x - x_2)^2}\Big) = q\frac{(q_1 + q_2)x^2 - 2q_1 x x_2 + q_1{}^2}{x^2(x - x_2)^2} \quad (2)$$

As the motion is invariant with respect to simultaneous change signs of all charges, we will always assume that $q > 0$. If $q_1 + q_2 \neq 0$, then the equations for critical points (where the force equals zero) are

$$x^2 - 2xQx_2 + Qx_2^2 = (x - Qx_2)^2 - Q^2x_2^2 + Qx_2^2 = 0, \quad Q = \frac{q_1}{q_1 + q_2}$$

whence the roots are

$$x_{\pm} = Qx_2 \pm x_2\sqrt{Q^2 - Q}$$

One can write also x_2 in terms of x

$$x_2^2 - 2xx_2 + Q^{-1}x^2 = (x_2 - x)^2 - x^2 + Q^{-1}x^2 = 0$$

$$x_{2.\pm} = x \pm x\sqrt{1 - \frac{q_1 + q_2}{q_1}} = x\Big(1 \pm \sqrt{-\frac{q_2}{q_1}}\Big)$$

Assuming that q_1, q_2 have different charges we have

$$Q^2 - Q = Q(Q - 1) = \frac{q_1}{q_1 + q_2}\Big(\frac{q_1}{q_1 + q_2} - 1\Big) = -\frac{q_1q_2}{(q_1 + q_2)^2} \geq 0$$

As the expression under root is positive, there always should be two real roots. Putting $z = -\frac{q_2}{q_1}$, we have

$$x_{\pm} = Qx_2\Big(1 \pm \sqrt{-\frac{q_2}{q_1}}\Big) = x_2\frac{1}{1 - z}(1 \pm \sqrt{z}) = x_2\frac{1}{1 \mp \sqrt{z}}$$

Note that the force cannot have more than 2 zeros on R. We consider all possibilities the followng possibilities:

1. $q_1q_2 > 0$. If particles 1 and 2 have the same sign, then it is clear that if $q_1, q_2 > 0$ then the particle will go to infinity. If $q_1, q_2 < 0$ then the particle escapes to ∞ if $v(0) > 0$ and $H(0) \geq 0$. Otherwise, it collides with particle 2.

2. $0 < q_1 < |q_2|$.

3. $-q_2 < q_1 < 0$.

4. $q_1 + q_2 = 0$. In cases 2,3,4 the force also cannot be zero on (a, ∞), and has the the same sign.

5. $0 < |q_2| < q_1$. Here the force has the only one root on (a, ∞). Moreover, $U(x) > 0$ and decreases for large x because $U(x) \to 0$ as $x \to \infty$. Also, $U(x) < 0$ for small $x - a$ and $U(x) \to -\infty$ as $x \to a + 0$. Thus, $U(x)$ has one maximum on (a, ∞) and the system cannot be stable.

6. $0 < q_2 < |q_1|, q_1 < 0$. Here $U(x) \to +\infty$ as $x \to a + 0$. Also $U(x) < 0$ for sufficiently large x and increases to 0 as $x \to \infty$. Thus $U(x)$ has exactly one minimum. It is clear that, for any fixed initial conditions, there exists such $C_1 > 0$ that $x(t) > a + C_1$. The escape to infinity is possible only if $H(0) \geq 0$. In fact, if at some moment t_1 the velocity $v(t_1) < 0$ then at some moment $t_2 > t_1$ the particle will come back to the same point but with velocity $v(t_2) = -v(t_1) > 0$. After this it will go straight to infinity iff $H(t_2) = H(0) \geq 0$. If $H(t_2) = H(0) < 0$ the velocity of the particle will become zero at the point y where $U(y) = H(0)$.

Case $0 < x(0) < a$ This case is easy and less interesting. Remind that we assumed that $q_3 = q > 0$.

1) If particles 1,2 have different signs, then particle 3 is attracted by one particle and is repelled by the other. Then it is evident that it will collide with one to which it is attracted.

2) $q_{,1}, q_2 < 0$. Then there is one unstable fixed point (maximum of the potential).

3) $q_{,1}, q_2 > 0$. Then there is one stable fixed point (minimum of the potential), and thus the set $\{(x(0), v(0)\}$ of initial conditions contains an open subset defining bound states.

Only one particle has infinite mass

Case $x_1(t) \equiv 0 < x_2(0) < x_3(0)$ Let the charges be $q_1 > 0, q_2, q_3$.

Proposition 2. Fixed (equilibrium) states exist iff $q_2 < 0, q_3 > 0$ and

$$|q_2| < q_3, q_1 = \frac{q_3}{(\sqrt{-q_3/q_2} - 1)^2} \tag{3}$$

All of them are unstable

Proof. Denote F_2, F_3 – forces on particles 2 and 3 c oorrespondingly. Then there are 4 cases:

1) $q_2, q_3 > 0$. Here F_3 is always positive. Moreover, particles cannot collide, then for any initial velocities, v_3 once becomes zero, and particle 3 goes to ∞;

2) $q_2, q_3 < 0$. Force F_2 on particle 2 is always negative. Thus, if for some t_0 $v_2(t_0) \leq 0$ the particle 2 collides with particle 1. Otherwise, $v_2(t)$ always tends to some $v_2(\infty) > 0$, and then $x_2(t)$ increases to $x_2(\infty) = \infty$;

3) $q_2 > 0, q_3 < 0$. Note that the force F_3 on particle 3 is always negative, and the force F_2 on particle 2 is always positive. It follows that $v_2(t)$ and $v_3(t)$ are monotone increasing and decreasing correspondingly. Thus, either the particles 2 and 3 will collide or particle 3 goes to infinity;

4) $q_2 < 0, q_3 > 0$. In this case there can be fixed states. They should satisfy two equations

$$F_2 = q_2\Big(\frac{q_1}{x_2^2} - \frac{q_3}{(x_3 - x_2)^2}\Big) = 0, \quad F_3 = q_3\Big(\frac{q_1}{x_3^2} + \frac{q_2}{(x_3 - x_2)^2}\Big) = 0$$

or equivalently, putting $z = \frac{x_2}{x_3} < 1$,

$$\frac{q_1}{q_3}\frac{1}{x_2^2} = -\frac{q_1}{q_2}\frac{1}{x_3^2} = \frac{1}{(x_3 - x_2)^2} \Longrightarrow \frac{q_1}{q_3} = -\frac{q_1}{q_2}z^2 = \frac{1}{(z^{-1} - 1)^2}$$

Thus

$$z = +\sqrt{-\frac{q_2}{q_3}}, q_1 = \frac{q_3}{(z^{-1} - 1)^2}$$

It follows that the conditions (3) are necessary and sufficient for the existence of continuum of fixed states. They satisfy the equation

$$z = \frac{x_2}{x_3} = +\sqrt{-\frac{q_2}{q_3}}$$

They are unstable because in the cone $\{(x_2, x_3) : 0 < x_2 < x_3\} \subset R^2$ the function $U(x_2, x_3)$ on each direct line $x_3 = \alpha x_2$, $\alpha = +\sqrt{-q_3/q_2} > 1$ has critical point, which is the maximum of U.

Case $x_1(0) < x_2(t) \equiv 0 < x_3(0)$ Introduce variables $y_1 = x_2 - x_1 > 0, y_2 = x_3 - x_2 > 0$ in the quarter-plane $R^2_+ = \{y = (y_1, y_2) : y_1 y_2 > 0\}$. We have two equations

$$F_1 = -\frac{q_1 q_2}{y_1^2} - \frac{q_1 q_3}{(y_1 + y_2)^2} = 0, \quad F_3 = \frac{q_3 q_2}{y_2^2} + \frac{q_1 q_3}{(y_1 + y_2)^2} = 0$$

If we assume $q_1 > 0$, it follows that

$$F_2 + F_3 = q_2\Big(-\frac{q_1}{y_1^2} + \frac{q_3}{y_2^2}\Big) = 0 \Longrightarrow \frac{q_1}{q_3} = \frac{y_1^2}{y_2^2} \Longrightarrow q_1, q_3 > 0, q_2 < 0$$

Then

$$\frac{q_2}{y_2^2} + \frac{q_1}{(y_1 + y_2)^2} = 0 \Longrightarrow -\frac{q_2}{q_1} = \frac{1}{(1 + \sqrt{-q_3/q_1})^2}$$

This is the condition for existence of fixed state. Now let us prove that if the critical point of the potential energy

$$U(y) = \frac{q_1 q_2}{y_1} + \frac{q_2 q_3}{y_2} + \frac{q_1 q_3}{y_1 + y_2}$$

exists, it is unique. It follows from the equations which uniquely define y_1, y_2. As $U \to -\infty$ if either $y_1 \to 0$ or $y_3 \to 0$, the critical point is the maximum of U.

All particles have finite masses Let the charges and coordinates of these particles be q_1, q_2, q_3 and $x_1 < x_2 < x_3$ correspondingly. The simplest example is the following: $q_{-1} = q, q_0, q_1 = q$ and $x_{-1} = -x < x_0 = 0 < x_1 = x$ correspondingly. Then such configuration is fixed iff

$$\frac{q^2}{4x^2} + \frac{q q_0}{x^2} = 0 \Longleftrightarrow q = -4q_0$$

In fact, this means that forces on the leftmost and rightmost particles are zero. The force on the middle particle is zero by symmetry.

In general also, if forces on particles 1 and 3 are zero, then the force on particle 2 is also zero. The equilibrium conditions are given by three equations for the forces on particles $-1, 1, 0$ correspondingly:

$$\frac{q q_{-1}}{x_{-1}^2} + \frac{q_1 q_{-1}}{(x_{-1} + x_1)^2} = 0, \quad \frac{q q_1}{x_1^2} + \frac{q_1 q_{-1}}{(x_{-1} + x_1)^2} = 0, \quad \frac{q q_{-1}}{x_{-1}^2} + \frac{q q_1}{x_1^2} = 0 \qquad (4)$$

One can see then when the solution of (4) exists.

Problem. For $N \geq 3$ particles in R^d provide a classification of all fixed configurations.

0.4 Systems of Atoms and Biological systems

Simplest system of atoms could be the following example with 4 particles with trajectories $x_i(t) \in R^2, i = 1, 2, 3, 4$. They form two atoms with particles $i = 1, 2$ and $i = 3, 4$ correspondingly. We say that these atoms are space independent if there are two convex nonintersecting open simply connected domains (for example, closed balls) Λ_{12} and Λ_{34} such that for any t: $x_1(t), x_2(t) \in \Lambda_{12}$ and $x_3(t), x_4(t) \in \Lambda_{34}$. Such systems cannot exist in Celestial Mechanics and the question is whether they exist in Coulomb mechanics.

The more intriguing question is whether it is possible for more complicated systems of atoms (long molecules) in domains $O_k, k = 1, \ldots, N$, with very large N looking like a chain or even more complicated graph. The far looking problem: what phenomena in biological systems can be described in the framework of (classical) Coulomb mechanics ?

Simplified problem Even simpler bounded trajectory could be as follows. In R^2 particle 1 stands still at the origin, that is $x_1(t) = 0$. The trajectory $x_2(t)$ of particle 2 stays always in some ellipse O_2 with centrum at the origin (that is the particle 2 rotates around particle 1). Particle 3 stays always in some circle O_3 with centrum at some point $(x, 0)$ on the x-axis. Important condition is that the radius of O_3 is less than $|x|$, or even more: O_2 and O_3 do not intersect.