# Numerical study of classical motions of two equal-mass opposite-charge ions in a Paul trap*

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Abstract

We conduct a numerical test of nonlinear stability, following Danby's definition and Nauenberg's implementation, of two oppositely charged, equal-mass ions in a Paul trap operated at a single frequency, as a function of initial conditions. We find a small, but non-negligible domain of stability in the space of trap parameters, which opens the door to experimental searches.

## Introduction

Numerous new few-body systems bound by the Coulomb potential *in vacuo* have recently been discovered in numerical searches, see Refs. [1, 2] and references therein. No such system can be detected in a terrestrial experiment, due to the presence of Earth's gravitational field, so their detection requires a confinement device, i.e., an ion trap, such as the Paul one, which, in turn, significantly impacts on the dynamics of the few-body system.

Paul traps have long been known to confine charged particles, ranging from atomic ions to macroscopic charged objects. The case of two, or more, oppositely charged, yet equal-mass ions has only recently been studied, however: Refs. [3, 4, 5] showed that it is possible to simultaneously confine

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opposite charge ions with markedly different charge-to-mass ratios in a Paul trap operated at two frequencies. It is the equal-mass limit of the two-body opposite-charge case in a single-frequency Paul trap that interests us here.

The question is if and when two equal-mass opposite-charge macroscopic particles' classical periodic orbit is stable in a Paul trap? It is not difficult to show analytically in the adiabatic limit that an electrically charged bound state of two opposite-charge, equal mass particles remains confined, though its center-of-mass may move around the trap, in a Paul trap operated at a single frequency. The case of electrically neutral bound states must be studied numerically, however, as they may, but need not become deconfined by the influence of the trap's field, depending on the precise values of the trap parameters and initial conditions of the pair.

In this note we present the results of a numerical investigation of the stability domain of two equal-mass, and equal, but opposite-sign charged macroscopic bodies periodic orbit in a Paul trap operated at a single frequency. We establish a nonlinear stability domain in the space of control parameters using the Danby-Nauenberg method [6, 7, 8].

## Preliminaries

The Keplerian elliptic periodic orbit is *marginally* linearly stable *in vacuo*, but not so in a Paul trap: the trap's time-variable electric field makes this system non-Hamiltonian. Therefore, only a numerical analysis can determine its stability. The nonlinear stability domain of solutions to the two-body problem was obtained by a numerical integration of the equations of motion, and then measuring whether, for a small initial deviation from the initial conditions, the orbit remains confined after some, sufficiently large number $n$ of periods. We found that $n \simeq 250 - 500$ was sufficient for a test of nonlinear stability, in agreement with similar conclusions by Nauenberg [8] in the case of Newtonian three-body systems [1].

The primary goal of this numerical simulation is to establish if and when the motion of the pair's center of mass (CM) is confined. Zero total charge of a pair suggests decoupling from the electric field and thus deconfinement, so we investigate that case as the critical one.

The simulations were implemented using the (standard) fifth-order Runge-Kutta algorithm. A Coulomb pair moving on a Keplerian elliptic orbit *in vacuo* has an intrinsic frequency $f$ (inversely proportional to the period $T$) associated with its size, or energy. The applied electric field in the Paul trap, on the other hand has its own (independent) frequency $f_0$. The ratio of these two frequencies (both of which are scale-dependent) represents one

[1] Nauenberg [8] showed that "this nonlinear stability domain looks surprisingly similar to the stability domain of the Mathieu equation with an additional nonlinear restoring or damping term" and that "a linear curve fits the lower part of the domain with a slope that is ... in good agreement with the numerical linear stability results of Danby [6] and Bennett [7]".

dimension in the space of scale-invariant parameters. The scale independent properties, such as the stability of the motion, can only depend on this ratio.

We have investigated the parameter space of initial conditions where the frequency $f$ of the free-space Keplerian orbit of the charged pair is comparable to the frequency $f_0$ of the applied field, i.e., when the system is close to resonance. Thus we study the most interesting case of strong coupling between Coulomb interaction and the "driving force" of the Paul trap field.

## Results

We have kept the mass of individual particles fixed at 1 AMU and the charge of the particles at $\pm 1e$. Both particles were initially placed on the $x$-axis, with equal velocities parallel to the $y$-axis, but in opposite directions (positive particle has $v_{y0} > 0$), thus ensuring that the particles were confined to $x - y$ plane. The $x$ coordinates and velocities of particles in any given simulation were chosen to correspond with the orbit (defined by the Coulomb interaction, without any external fields) that has a predefined nominal rotation frequency $f$.

The longest-lived orbits were observed starting from the center of the trap. We scanned a region of initial conditions with nominal rotation frequencies $f$ ranging from $0.6f_0$ to $2.2f_0$, with $f_0 = 2$ MHz being the frequency of the applied field. By fixing this specific value of the driving force frequency, we have also set the length scale (in millimeters).

The second parameter over which the initial conditions were scanned is the displacement of the particle pair from the center of the trap. The displacement is equal to the starting $x$-coordinate of the particle center of mass. The total length of time in each simulation is $125\mu s$, which represents 250 periods of the applied field. Then, we displaced the particles from the center of the trap and measured how much longer the bound motion of the charged pair was observed. We have calculated, as a measure of stability, the number of cycles (rotations in the center of mass frame) completed during one simulation run, see Fig. 1. We performed 2400 simulations in total.

It should be immediately apparent in Fig. 1 that for displacement values larger than $1.2mm$, the trapping field tears the pair apart and the particles continue on as individually trapped charges. For lower values of displacement, however, we observe a non-trivial structure with three distinct regions.

1) The first, the "least stable" (dark green to blue) region with 150-200 completed rotations centered on $f/f_0 = 1$ extends the furthest, out to $1.2mm$ of displacement. Note that, although this is not directly visible in this graph, we have checked that all of the trajectories in this region ended breaking up before the simulation completed (after roughly $80\mu s$).

2) In the second (light green) region, up to $0.5mm$ of displacement and around $f/f_0 = 1$, the particles actually remained bound by the Coulomb

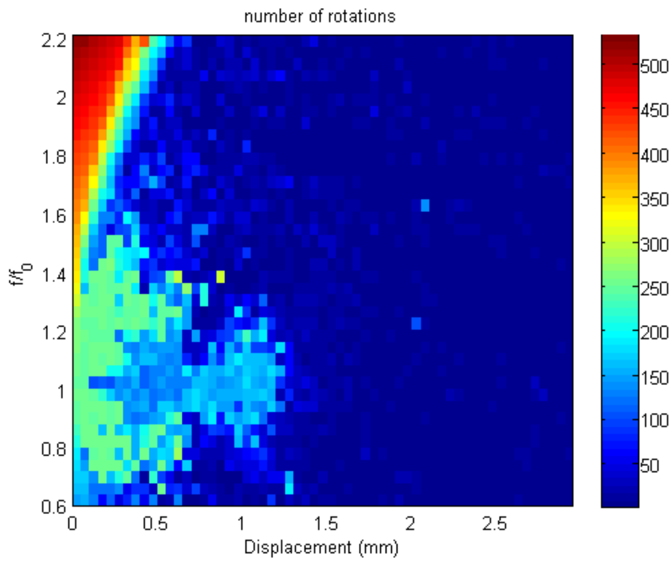


Figure 1: (color on-line) The number of completed periods/rotations (see color code on the right-hand side) in the CM reference frame as a function of the initial displacement from the center of the trap (in mm, on the x-axis) and of the frequency ratio $f/f_0$ (on the y axis). The conditions in the upper left-hand corner of the graph (dark red) allowed for two times higher rotation count when driven by two times higher frequency, with the region of acceptable displacement growing with the frequency of the applied field.

interaction for the duration of the simulation completing their nominal 250 rotations.

3) Finally, the third (yellow to red) region is that of higher frequency ratio $f/f_0 \geq 1.5$ (the upper left-hand-side corner) that has a significantly higher count of completed orbits $n$. Given that the nominal frequency $f$ is higher than $f_0$ in this region, an increase of the number of completed orbits would be expected on this account alone, but, more interestingly, the region of stability expands with the increasing frequency ratio $f/f_0$, thus indicating that pairs with rapidly rotating orbits "feel" the effects of the Paul trap field to a lesser extent than the slower rotating ones. It is in this region that one should try and conduct experiments.

## Conclusions

In this paper we have investigated the nonlinear stability of electrically neutral equal-mass two-body periodic orbits in a Paul trap. As the Paul trap's electric field depends on time, and is generally not spherically symmetric, the angular momentum and energy are not conserved, thus eliminating two integrals of motion. Consequently, a test of stability of periodic solutions to equations of motion had to be purely numerical.

Our numerical stability calculations show that a small, yet clearly outlined domain exists in the space of parameters of a Paul trap, where a Kepler-like motion of pair of opposite-charged ions is nonlinearly stable and where observation of such a periodic Coulomb 2-body orbit is likely.

The present study is meant to invite an experimental observation of such motion, which should be a precursor to similar investigations of periodic systems with three, or more charged particles, such as those in Refs. [1, 2], moving in a Paul trap.

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