

Nonlinear Ion Trap Stability Analysis

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Abstract.

This paper investigates the dynamics of an ion confined in a nonlinear Paul trap. The equation of motion for the ion is shown to be consistent with the equation describing a damped, forced Duffing oscillator. All perturbing factors are taken into consideration in the approach. Moreover, the ion is considered to undergo interaction with an external electromagnetic field. The method is based on numerical integration of the equation of motion, as the system under investigation is highly nonlinear. Phase portraits and Poincaré sections show that chaos is present in the associated dynamics. The system of interest exhibits fractal properties and strange attractors. The bifurcation diagrams emphasize qualitative changes of the dynamics and the onset of chaos.

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1. Introduction

Quadrupole ion traps [1, 2] have proven to be an extremely versatile tool in atomic physics, high-precision spectroscopy, fundamental tests on quantum mechanics concepts [3], quantum metrology, physics of quantum information, studies of chaos and integrability for dynamical systems, mass spectrometry [4], quantum optics and studies of non-neutral plasmas [5, 6, 7, 8].

Deterministic chaos deals with long-time evolution of a system in time. A system evolving in time is a dynamical system. Chaos is related to the study of the dynamical systems theory [9, 10] or nonlinear dynamics [11, 12, 13, 14]. Dynamical systems can be either conservative, case when no friction is present and the system does not lose energy in time, or dissipative, when it loses energy in time thus approaching some asymptotic or limiting condition [15]. That asymptotic or limiting state, under certain conditions, is where chaos occurs. We can ascertain that chaos occurs in deterministic, nonlinear, dynamical systems. Other chaos-related geometric objects, such as the boundary between periodic and chaotic motions in phase space, also may have fractal properties.

A nonlinear chaotic system, the parametrically kicked nonlinear oscillator, may be realised in the dynamics of a trapped, laser-cooled ion, interacting with a sequence of standing wave pulses [16]. We investigated ion dynamics in a nonlinear quadrupole Paul trap with octupole anharmonicity. The system is dissipative. Ion dynamics is described by a nonlinear Mathieu equation. All perturbing contributions have been taken into account (damping, multipole terms of the potential, harmonic excitation force). In order to complicate the picture and approach real conditions, we have also considered that the ion undergoes interaction with a laser field. The resultant equation of motion can be considered as a perturbed Duffing type equation, which is a generalization of the linear differential equation that describes damped and forced harmonic motion.

2. Equation of motion for an ion confined in a nonlinear trap

We studied the case of an ion confined in a quadrupole nonlinear Paul trap, which we treated as a time-periodic differential dynamical system. Dissipation in such system is very low, which leads to a number of interesting phenomena. The equation of motion along the x direction, for a particle of electrical charge Q and mass M , which undergoes interaction with a laser field in a quartic potential $V(u) = \mu u^4$, $\mu > 0$ and in presence of damping [17], can be expressed as

$$\frac{d^2u}{d\tau^2} + \gamma \frac{du}{d\tau} + [a - 2q \cos(2\tau)]u + \mu u^3 + \alpha \sin u = F \cos \omega_0 t, \quad (1)$$

where $u = kx$, $\tau = \Omega t/2$, $\alpha = 2k^2\Omega_0 \cos \theta / M\Omega^2$, γ and μ are the damping and the anharmonicity coefficient respectively, while the adimensional parameters are expressed as $a = -8QU_0/M\Omega^2d$ and $q = 4QV_0/M\Omega^2d$, with $d = r_0^2 + 2z_0^2$. For a typical Paul Trap $a = 0.1$ and $q = 0.7$. The micromotion frequency is denoted by Ω , U_0 and V_0 are the static and time-varying trapping voltages, r_0 and z_0 are the trap semiaxes, while Ω_0 is the Rabi frequency for the ion-laser interaction and $\cos \theta$ is the expectation value of the x projection

spin operator for the two level system with respect to a Bloch coherent state. The expression $F \cos \omega_0 t$ stands for the driving force, an external excitation at frequency ω_0 .

Eq. 1 can also be viewed, in a good approximation, as Newton's law for a particle in a double-well potential. The force $F \cos \omega t$ is an inertial force that arises from the oscillation of the coordinate system. The mathematical analysis of the Eq. 1 (which is dimensionless) requires some advanced techniques from global bifurcation theory [9, 10, 11, 12, 13, 14].

Our modest goal was to gain some insight into Eq. 1 through numerical simulations. The dynamical behavior of the equation of motion we considered is studied numerically by varying the damping and the driving frequency parameters, as well as the amplitude parameter. We finally discuss the possibility of observing chaos in such a nonlinear system [18]. Chaotic regions in the parameter space can be identified by means of Poincaré sections [9, 10, 12, 13, 15].

3. Phase space orbits for the nonlinear parametric oscillator. Poincaré sections. Chaos and attractors

The ion can be considered as a forced harmonic oscillator, described by a nonautonomous or time-dependent equation of motion. Forced oscillators have many of the properties associated with nonlinear systems. Most nonlinear systems are impossible to solve analytically. The trajectory represents the solution of the differential equation starting from an initial condition. A picture which shows all the qualitatively different trajectories of the system, is called a phase portrait. The appearance of the phase portrait is controlled by the fixed points. In terms of the original differential equation, fixed points represent equilibrium solutions. An equilibrium is considered as stable if all sufficiently small disturbances away from it damp out in time.

We have performed a numerical integration of the equation of motion, using the fourth order Runge-Kutta method [19]. In order to illustrate the dynamics of the trapped ion we have represented the trajectories in the two-dimensional phase space (phase portraits) [19] and extended phase space as seen in Fig. 1, with an aim to emphasize the regular and chaotic orbits.

Studying the associated phase portraits we observe that the cubic term $-\mu u^3$ provides a nonlinear restoring force at large x , while the linear term pushes away from the origin. In addition, there is the usual velocity-proportional damping. The potential for this oscillator has a double-well structure. For certain initial conditions, there is an unstable equilibrium point at $x = 0$, and given some damping the particle has to fall into one side of the well or the other if it approaches the equilibrium point with just enough energy to move over it. The homogeneous problem (non-driven oscillator) has no surprises in it. Given an initial condition there is a unique phase-space trajectory that leads to the particle winding up at the bottom of one of the two wells after the mechanical energy is converted to heat. When the oscillator is driven by a periodic force the system can reach a limit cycle, where as much mechanical energy is lost per cycle as is dumped into the system by the crank. Chaos appears as a result of the two wells connected by the unstable equilibrium point.

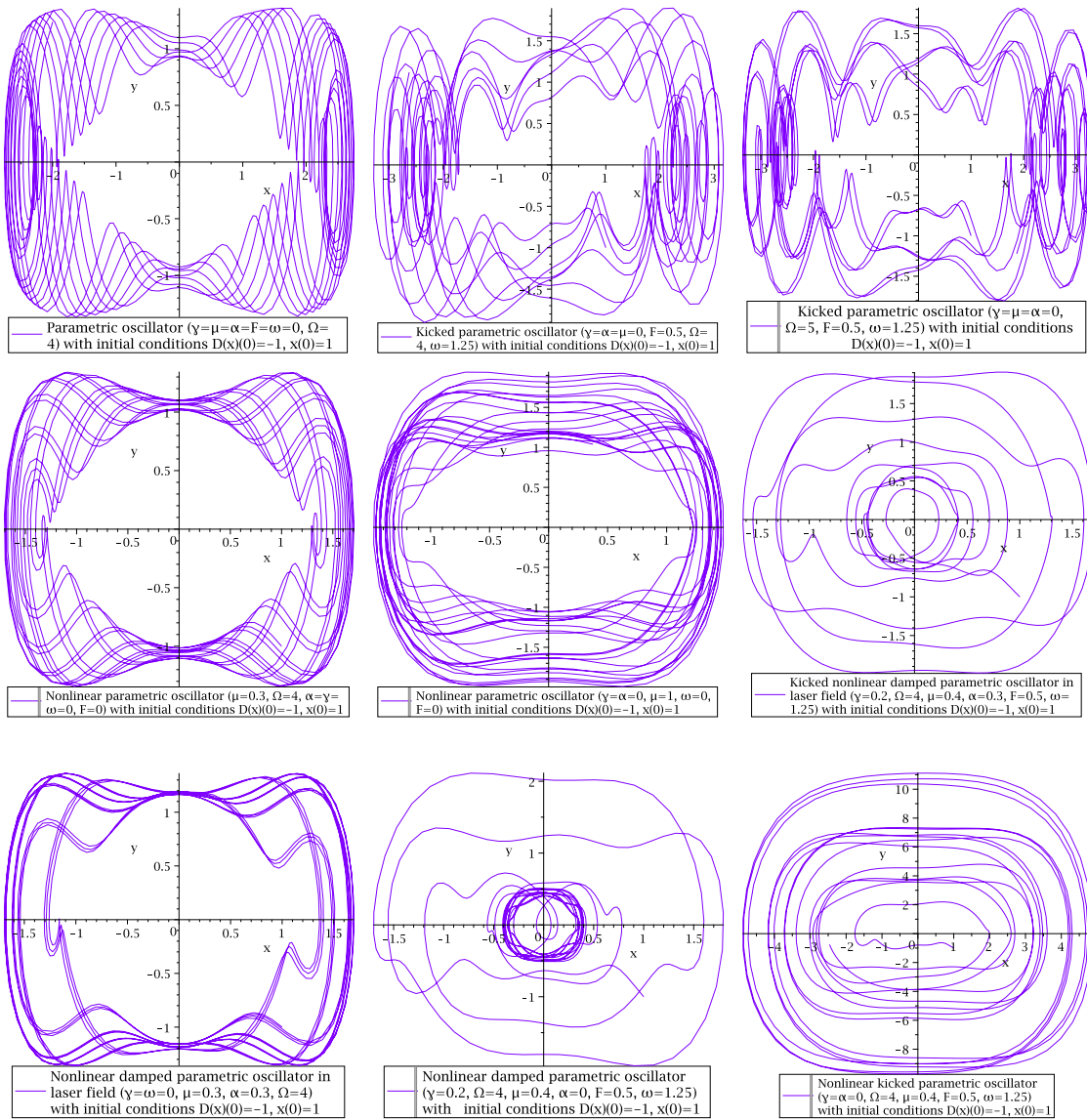


Figure 1. Phase space orbits for an ion confined within a nonlinear trap

The phase portraits clearly reflect the existence of one or two attractors and of fractal basin boundaries for the trapped ion, assimilated with a periodically forced double well oscillator. For some of the parameter values presented in Fig. 1, the system has two periodic attractors, corresponding to forced oscillations confined to the left or right well. Depending on the initial conditions, the system can converge rapidly to one of the two attractors. Frequency doubling is also present, which represents a stage in the passage from ordered dynamics to a chaotic one. The basins of attraction generally have a complicated shape, and the boundary between them is fractal [20]. As it can be seen, there are cases when the dynamics exhibits periodicity.

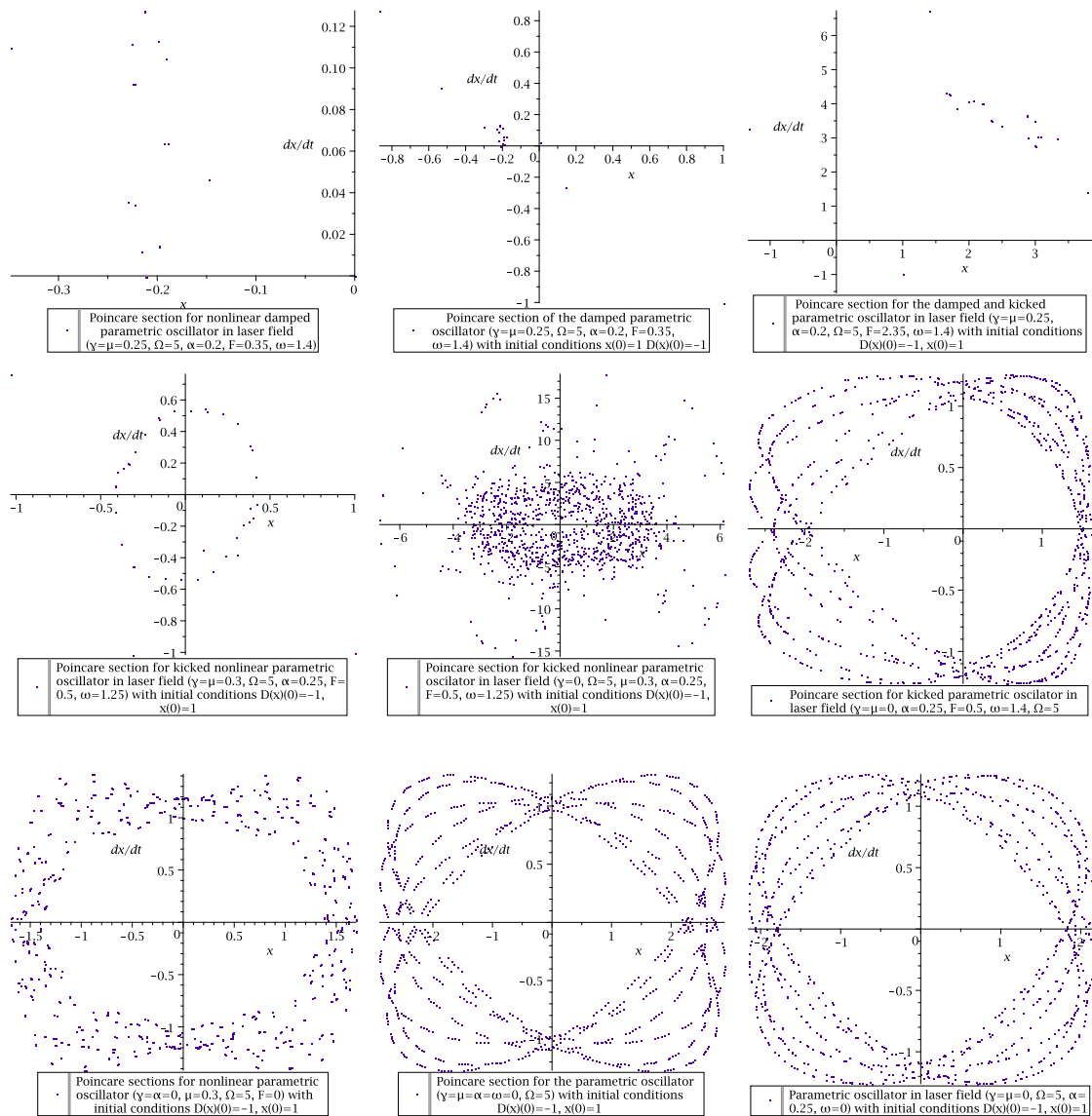


Figure 2. Poincaré sections for an ion confined within a nonlinear trap

The Poincaré sections are represented in Fig. 2. As it can be seen, depending on the values of the control parameters we choose, the Poincaré sections describe regular motion, the transition from chaos to order or reflect the existence of chaos, in a large number of cases. We emphasize on the appearance of what we consider to be strange attractors. A strange attractor represents the limiting set of points to which the trajectory tends (after the initial transient) every period of the driving force. Figs. 2 a – d describe regular motion, we have points or cluster of points, or a fractal set in case e. The structure that appears in the Poincaré section in cases e and g case can be proven to be a complicated curve, namely a fractal. This leads to the name strange attractor for this oscillator, which is an indication that the system is chaotic. Chaos prevails too in the other cases, but the system exhibits periodic orbits.

From calculus, we can ascertain that the frontiers of the stability diagram are shifted

towards negative regions of the a axis in the plan of the control parameters (a, q) as already reported by Sevugarajan [21].

In order to ease understanding of the phenomena involved, we have represented the phase portraits, Poincaré sections and bifurcation diagrams for the driven, damped Duffing oscillator in Fig. 3 as well as for an ion confined in the trap, both in absence and presence of laser field, as seen in Fig. 4, Fig. 5 and Fig. 6. In case of the damped Duffing oscillator, plots of $x(t)$ and $y(t)$ show that both exhibit aperiodic appearance. The system is chaotic, at least for the chosen initial conditions. $x(t)$ changes sign frequently, which means that the particle crosses the hump repeatedly, as expected for strong forcing. Due to the fact that we deal with a non-autonomous system, Fig. 3 is not a true phase portrait. The state of the system is described by the triplet (x, y, t) , not only (x, y) alone. In order to compute the system's subsequent evolution, all three variables are required. The associated phase portrait should be regarded as a two-dimensional projection of a three-dimensional trajectory. The tangled appearance of the projection is typical for non-autonomous systems, the basins of attraction are evident [12].

A more detailed insight results from the Poincaré section, which results by plotting $(x(t), y(t))$ whenever t is an integer multiple of 2π . Practically, we strobe the system at the same phase for each drive cycle. Looking at the Poincaré section, we observe that the points fall on a fractal set, which we interpret as a cross section of a strange attractor for Eq. 1. The successive points $x(t), y(t)$ are found to hop erratically over the attractor, while the system exhibits sensitive dependence on the initial conditions, which is the signature of chaos.

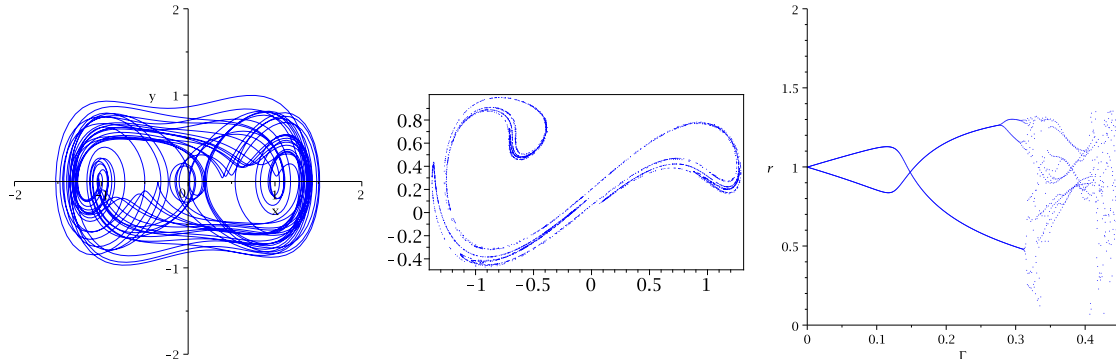


Figure 3. Phase portrait, Poincaré sections and bifurcation diagram for the Duffing oscillator. The values of the parameters are $\gamma = 0.3, \omega = 1.25, F = 0.5, \alpha = 1$. The bifurcation diagram corresponds to $0 < F < 0.5$

Figure 4 refers to an ion trapped in absence of the laser radiation. The phase portrait clearly depicts the existence of what seems to be a stable equilibrium (an attractor) and break of symmetry. The Poincaré section is made of a few dispersed points, chaos is absent. From the bifurcation diagrams, we can observe a period-doubling bifurcation, when increasing the value of the kicking term $F \geq 0.63$. Practically, frequency doubling is the route to chaos. When $0.85 \leq F \leq 1.8$ we have a mixture of order and chaos, with chaos prevailing. For $F > 1.9$ the system is no longer chaotic.

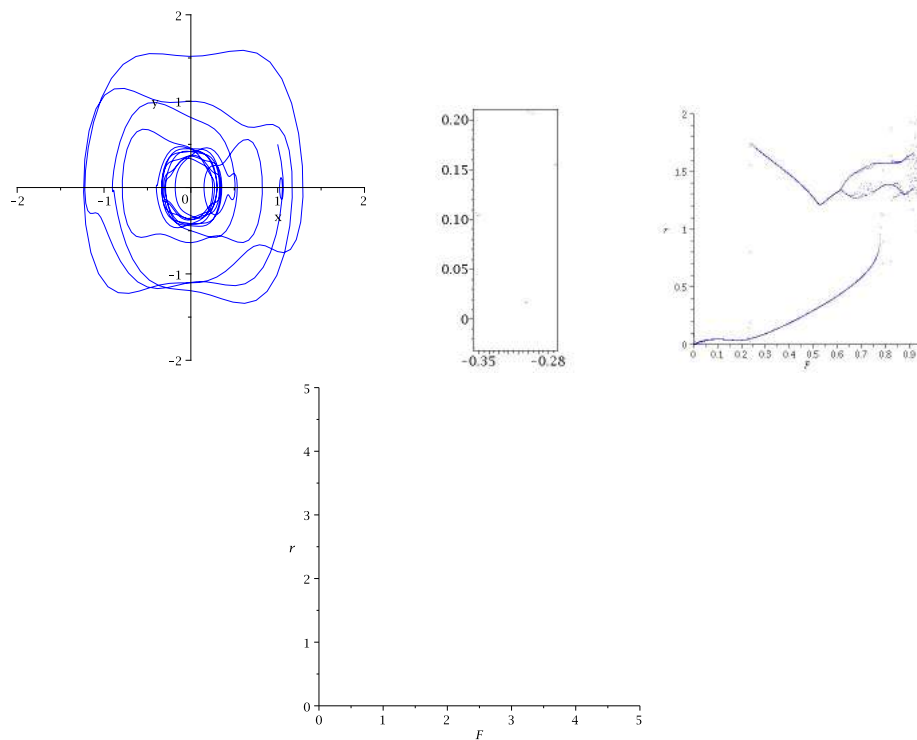


Figure 4. Phase portrait, Poincaré section and bifurcation diagrams for an ion confined in a nonlinear Paul trap. The values of the control parameters in Eq. (1) are $\gamma = 0.3, \omega = 1.25, F = 0.5, \mu = 1, \alpha = 0$. The first bifurcation diagram corresponds to $0 < F < 1$ while for the second diagram $0 < F < 5$

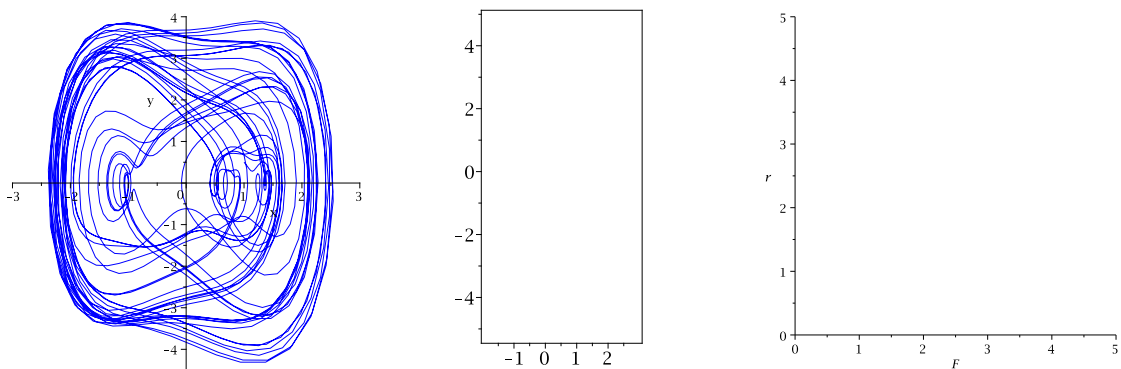


Figure 5. Phase portrait, Poincaré section and bifurcation diagram for an ion confined in a nonlinear Paul trap, in presence of laser radiation. The values of the control parameters in Eq. (1) are $\gamma = 0.3, \omega = 1.25, F = 2, \mu = 1, \alpha = 0.3$. The bifurcation diagram corresponds to $0 < F < 4$

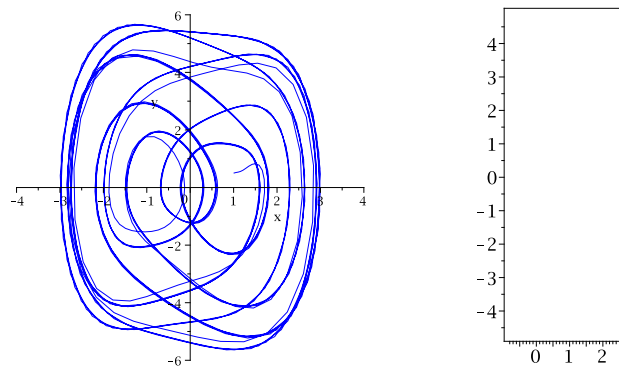


Figure 6. Phase portrait, Poincaré section for an ion confined in a nonlinear Paul trap, in presence of laser radiation. The values of the control parameters in Eq. (1) are $\gamma = 0.3$, $\omega = 1.25$, $F = 3$, $\mu = 1$, $\alpha = 0.3$.

In case of a trapped ion in presence of laser radiation, shown in Fig. 5, the phase portrait illustrates the existence of two attractors, which seem to be periodic. We can discuss about forced oscillations confined to the right or left well, because two basins of attraction appear. The points on the Poincaré section fall on a fractal set, which again is the signature of chaos. Thus, laser radiation renders the motion chaotic. The bifurcation diagram shows a period-doubling bifurcation for $F \approx 0.7$ and a mixture of order and chaos for $0.85 \leq F \leq 1.9$. For larger values of the kicking term, ion dynamics is ordered. The system exhibits dependence on the initial conditions, which is reflected in Fig. 6, where the phase portrait reflects the existence two attractors (two basins of attraction). The Poincaré section shows the dynamics to be periodic and ordered, without presence of chaos.

4. Conclusions

We have performed a qualitative investigation on the dynamical stability of an ion confined within a nonlinear quadrupole Paul trap, with anharmonicities resulting from the presence of higher order terms in the series expansion of the electric potential. The system exhibits a strongly nonlinear character. Damping and interaction with laser radiation were taken into account. A periodic kicking term was also considered. The stability of this dynamical system was investigated using numerical simulations and graphical illustrations. Phase portraits (orbits in the phase space) and Poincaré sections were obtained. Regular and chaotic regions of motion are thus emphasized in ion dynamics. System dynamics is chaotic when long-term behaviour is aperiodic.

For particular initial conditions, some of the solutions obtained present a certain degree of periodicity, although the dynamics is irregular. We show that the damped parametrical oscillator exhibits fractal properties and complex chaotic orbits. This problem can also be related to the subject of deterministic chaos, as fully deterministic systems can provide chaotic behaviour. Chaotic (fractal) attractors were identified for particular solutions of the equation of motion. The motion on the strange attractor exhibits sensitive dependence on initial

conditions. This means that two trajectories starting very close together will rapidly diverge from each other, and will show utterly different behaviour thereafter. Strange attractors are often fractal sets.

It is often more meaningful to characterize systems possessing complex dynamics through certain quantities involving asymptotic time averages of trajectories. Examples of such quantities are power spectra, generalized dimensions, Liapunov exponents and Kolmogorov entropy. Under certain conditions such quantities can be calculated in terms of averages of periodic orbits.

5. Acknowledgements

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