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An Introduction to Chaos in dynamic Ion Traps

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Abstract

Concepts in nonlinear dynamics and chaos are discussed on an introductory level. Chaos is shown to play a major role in the physics of the Paul trap and the dynamic Kingdon trap.

1. Introduction

Chaos, just another one of these modern fads that has reached its peak and will go away soon? Not at all. First, chaos has a history longer than the history of quantum mechanics [1, 2], and permeates the solar system [3, 4] as well as just about any other branch of the natural sciences. Second, chaos is not only ubiquitous, chaos is also "fundamental" with implications that upset many, not only the weather man. For short, chaos is here to stay. In physics chaos not only stood its ground but its importance increases as more and more systems are found to exhibit instabilities typical of chaotic motion. Even quantum mechanics had to acknowledge its existence. Many strong-field atomic physics effects for instance, difficult to explain in the traditional language of quantum perturbation theory, become "natural" and "physical" when expressed in the language of nonlinear dynamics [5]. Recently, chaos emerged in an innocuous spectroscopic tool, the Paul trap [6, 7], and manifested itself in a host of novel nonlinear phenomena [8–11]. The most impressive ones are melting and crystallization transitions [8–16]. Chaos was also identified in a dynamic version of the Kingdon trap [17].

No doubt, chaos is important, and it is important for ion trap physics. But what exactly is chaos? And how does it manifest itself?

This lecture gives some answers on an elementary level. It is based on a number of excellent review articles and books on nonlinear dynamics and chaos [1, 2, 18–24]. After introducing the basic concepts in Sections 2, 3 and 4, some manifestations of chaos in ion traps are discussed in Sections 5 and 6.

2. A brief history of chaos

It was clear to the ancients that chaos rules our planet. But what about the heavens? Everything there seems to be regular. Ptolemy tried to reproduce the apparent celestial regularity with his theory of epicycles. But more and more epicycles were necessary to describe the motion of celestial bodies. Did he try to expand in regular cycles what is really chaotic? But let us go slow.

Kepler (1571–1630) was firmly convinced that the solar system evolves in a regular, well ordered way. He is the author of "Harmonices Mundi" which liberally translated means "Cosmic Harmonies". He is also the author of a theory that relates the diameters of planetary orbits and indeed the very number of the planets to the regular Platonic bodies. His main scientific achievement is a detailed analysis of the orbit of Mars. Based on Tycho Brahe's (1546–1601) observational data he concluded that Mars, and all the other planets, traverse perfectly regular elliptical orbits. Thus, Kepler was certainly a proponent of order in the solar system.

Let us see what Sir I. Newton (1643–1727) had to say. Because of his law of universal gravitation, it was unlikely that the planets move on such perfect orbits as Kepler's ellipses. According to Newton, the planets interact not only with the sun, but also amongst each other, which leads to orbit distortions. In despair, after years of unsatisfactory numerical and analytical work, he postulated "periodic divine interventions" which were supposed to put the planets back on course after, according to his calculations, they had to be hopelessly off course. Therefore, it seems that Newton was not a champion of "order" in the solar system.

A similar opinion was shared by Leonhard Euler (1707–1783), who thought that accurate predictions on the future of the solar system are impossible. At one point, unable to satisfactorily reproduce the motion of the moon, Euler even thought that Newton's inverse square law of the gravitatial force may not be accurate and is to be blamed for the deviations.

The young philosopher and mathematician Pierre Simon de Laplace (1749–1827) was not impressed by the difficulties. He started his investigations on the stability of the solar system in 1773, then only 24 years old. He used perturbation expansions and soon pronounced proudly that the solar system is stable. According to his calculations, planetary orbits are certainly not as regular as Kepler's ellipses, but (in modern parlance) a Fourier transform of their motion consists of a countable set of discrete frequencies only. This means that according to Laplace the motion of the planets is quasi periodic and excludes the occurrence of any major catastrophies, such as planetary collisions.

Laplace went even one step further, a step which proved to be more influential than his "proof" of the stability of the solar system itself. Encouraged by his success he was led to an interpretation of Newton's equations which came to be known as *determinism.* Laplace's determinism states that given all the coordinates and momenta of all the particles in the universe at some instant of time t_0, the future and the past of the universe can in principle be predicted. Thus, he is the author of the "clock work" interpretation of the universe which became important as one of the philosophical driving forces behind the industrial revolution of the 18th and 19th centuries. Therefore, according to Laplace, we have the equation

$$\text{Laplace: Determinism} \Rightarrow \text{Predictability.} \qquad (1)$$

This interpretation of Newton's equations was challenged only about a century later and about a century ago by the eminent French mathematician and theoretical physicist Henry Poincaré (1854–1912). In a prize-winning essay on the occasion of King Oscar II's 60th birthday he concluded that already the gravitational three-body system is not analytically solvable in general, and that it can exhibit a complexity that is beyond imagination. Poincaré also found that orbits with slightly different initial conditions will diverge exponentially in such a situation. Because of the complexity and the exponential divergence of nearby orbits we now know that (1) is in general incorrect and has to be replaced by

$$\text{Poincaré: Determinism} \nRightarrow \text{Predictability.} \quad (2)$$

Thus, the theory of chaos was born.

For lack of visual aids, Poincaré's work did not impress many of his contemporaries. Only a few scientists continued Poincaré's seminal work. Amongst them, e.g., Birkhoff, Bogolyubov, and Mitropolskij. It was only in the 60's that Kolmogorov, Arnol'd and Moser proved the central theorem of nonlinear dynamics, now known as the KAM theorem [18, 19].

Still, nonlinear dynamics and "the theory of dynamical systems", as it was then called, remained a specialty subject for a hand-full of mathematicians. Not even the fundamental discovery of Edward Lorenz on the instability of the weather [25] made any impact. This situation finally changed when, in 1975, T.-Y. Li and J. Yorke published their paper "Period Three Implies Chaos" [26]. Although the theorem referred to in the title of Li and Yorke's paper was proved in much more generality more than eleven years before by the mathematician A. N. Sarkovskii [27], the name "chaos" stuck and defined the starting point of the "popular movement" in dynamical systems theory. Therefore, Li and Yorke's paper can be credited with bringing the subject of nonlinear systems theory to the attention of a wide scientific audience. The result was a dazzling proliferation of fundamental theorems and chaos scenarios in the late seventies and throughout the eighties that continues unabated. An indication of this situation may be a (most likely very incomplete) survey of the literature conducted with a PC based data base system that indexes some of the major current physics journals. For the years 1989–1992 a request to display all articles with the key words "chaos" or "chaotic" in their titles came up with 1206, 1403, 1518 and 1910 articles, respectively. A similar search for the key words "quantum chaos" or "quantum chaotic" came up with 31, 53, 45 and 105 articles. This illustrates the still growing importance of chaos.

But what about the chaoticity of the solar system? We left the subject with Poincaré and his analytically derived indications for the existence of chaos in the three-body problem. In the meantime the question of the stability of the solar system was attacked by several research groups with powerful computers. G. J. Sussman and J. Wisdom, e.g., used dedicated computers, such as the "digital orrery" and the "super computer tool kit" to establish that the time evolution of the whole solar system is chaotic [28]. J. Laskar [29] and J. Laskar, T. Quinn and S. Tremaine [30], using a combination of algebraic and numerical techniques, arrive at the same conclusion. The rate of exponential divergence, λ, of initially close orbits varies for different planets of the solar system, but is usually in the range $(5 \times 10^6\,\text{y})^{-1}$ to $(20 \times 10^6\,\text{y})^{-1}$. This means that the separation between initially close planetary trajectories grows by a factor $e = 2.718\ldots$ every 5 to 20 million years.

What does this mean in practice? Knowing the positions of the planets in the past would be extremely helpful for testing hypotheses on planetary capture, such as one of the theories of the origin of the moon or the origin of the planet Pluto. Also, exact planetary positions in the past could be used to test theories of climate. So, suppose somebody wants to know the positions of the planets at a time t, say, 1 billion years in the past. He is willing to spend an enormous amount of computer time on the project and has some source that provides him with the exact planetary momenta and the present planetary positions to an accuracy of 1 mm (!). In order to estimate a lower limit for the uncertainty in position accrued over 1 billion years, we use the "benign case" $\lambda = (20 \times 10^6\,\text{y})^{-1}$. Now, λ really characterizes the instability of trajectories in phase space. But assuming that the instability in position space is also roughly described by λ (which should not be too far off the mark), the initial uncertainty of 1 mm in the position will grow to an uncertainty of $\exp(10^9/20 \times 10^6)\,\text{mm} = 5 \times 10^{18}\,\text{m}$ over 1 billion years. This is just about a million times the diameter of the solar system, or about 500 light years! For obvious reasons this number should not be taken too seriously. But it gives a vivid impression of the seriousness and potential consequences of exponential instabilities and chaos. Specifying the initial conditions to 1 Å (the approximate size of a hydrogen atom) helps, but not much. Still, the tiny initial uncertainty will blow up to $5 \times 10^{11}\,\text{m}$ after 1 billion years. This corresponds to about three times the distance of the earth from the sun.

What this result tells us is significant. Due to the presence of chaos in the solar system, there is no way of knowing the positions of the planets with any certainty for a time 1 billion years in the past or in the future. Thus, based on dynamical considerations alone, it may never be known whether the moon or Pluto were captured at some time in the past.

Where does chaos come from? The answer, ultimately, lies in the properties of the continuum. If space and time were "grainy" such that mechanical systems could be found only in a countable number of states, all deterministic time evolution would ultimately be periodic with "chaotic" properties showing only transiently.

One of the most important questions is whether systems as complicated as the solar system are necessary for chaos to emerge. The answer is that chaos is possible in systems as simple as autonomous Hamiltonian systems with two degrees of freedom. For explicitly time dependent systems, even one degree of freedom is enough for chaos to emerge. One possible route to chaos, the period doubling route, is illustrated in the following section.

3. The logistic mapping: a model for chaos

Consider the mapping

$$x_{n+1} = qx_n(1 - x_n). \quad (3)$$

This mapping contains one control parameter q. It is interesting to investigate the behavior of the iterates x_n in the limit of large n for given control parameter q. The result of this analysis is usually presented in the form of a diagram

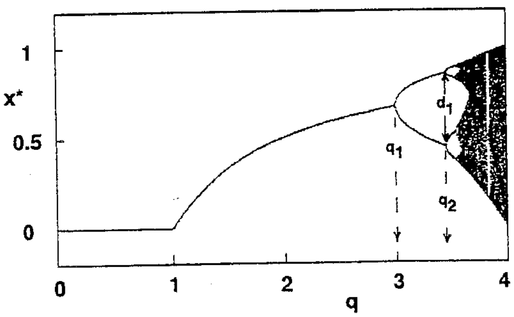

Fig. 1. Bifurcation diagram of the logistic mapping showing a period doubling route to chaos. The first two period doubling bifurcations are marked. They occur at $q_1 = 3$ and $q_2 = 1 + \sqrt{6}$, respectively.

such as the one shown in Fig. 1. It shows the asymptotic behavior of x_n, denoted by x^*, *vs.* the control parameter q. Let us see how x^* behaves as we scan the control parameter q. For $q < 1$ nothing special happens. The iterates of eq. (3) are attracted to $x^* = 0$. The situation is not much different for $1 < q < 3$. This time the iterates are attracted to $x^* = 1 - 1/q$. Something interesting happens at $q_1 = 3$. Here, the asymptotic values of x_n hop from one value to another. A bifurcation has occurred. Figure 1 shows that this scenario repeats at $q_2, q_3, \ldots$, until at some finite $q_\infty = q^* < 4$ the periodic behavior gives way to chaos. The bifurcation points q_j can also be interpreted as the critical points that mark the onset of period doublings in the logistic mapping. Therefore, the logistic mapping displays a period-doubling route to chaos. According to Feigenbaum [31] the ratio

$$\delta = \lim_{n\to\infty} \frac{q_n - q_{n-1}}{q_{n+1} - q_n} = 4.6692\ldots \tag{4}$$

is *universal*. It appears in many systems that show a period doubling route to chaos. The same is true for the ratio

$$\alpha = \lim_{n\to\infty} \frac{d_n}{d_{n+1}} = 2.50\ldots, \tag{5}$$

where the d_n are the maximal splittings of the bifurcation forks before the next bifurcation (see Fig. 2). Period doubling bifurcations reminiscent of the Feigenbaum scenario

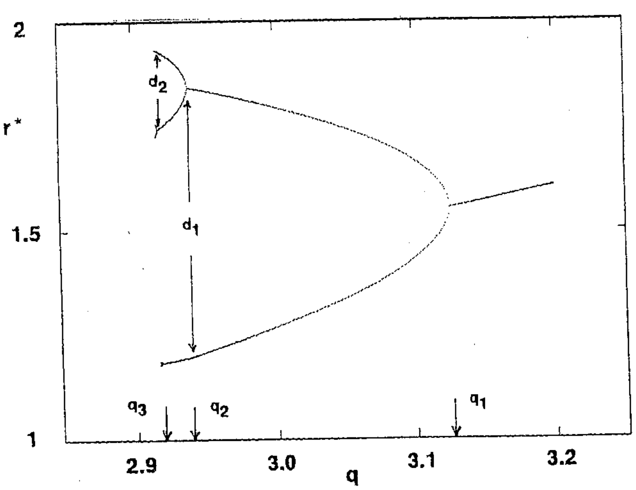

Fig. 2. Period doubling route to chaos for a single ion in the dynamic Kingdon trap. Period doubling bifurcations occur at $q_1 \approx 3.12$, $q_2 \approx 2.94$ and $q_3 \approx 2.917$. The splittings, d_1 and d_2, of the first and second fork are also shown.

were recently discovered in the dynamic Kingdon trap [17] (see Section 6).

4. Quantum chaos

Einstein was the first to appreciate that classical systems that do not possess the full set of constants of the motion, i.e., potentially chaotic systems cannot be quantized in a straightforward way [32]. Based on Poincaré's work on the three-body system [2] he points out that in this case the quantization rules of Sommerfeld and Epstein break down. Thus, classically chaotic systems such as the helium atom, presented a puzzle to the "old" quantum mechanics. The problem was not solved until the advent of the "new" quantum mechanics created by Heisenberg, Born, Jordan and Schrödinger. Although a powerful tool for the description of low lying quantum states, the semiclassical limit of classically chaotic systems is still not properly understood and is the topic of much of contemporary research in quantum mechanics. In fact, semiclassical quantization rules for chaotic systems were not known until the work of Gutzwiller who introduced periodic orbit expansions [19].

The existence of classical chaos provokes the question whether the typical traits of chaos, such as exponential instabilities and complexity, are present also on the quantum level. This question led to the modern field of quantum chaos research. I believe that there are essentially three main branches of this type of research which I call Type I, II, and III.

Type I research deals with the quantum signatures of chaos in classically chaotic systems. It is especially well developed in the case of autonomous Hamiltonian systems and periodically forced systems. Its main results concern the statistical properties of energy and quasi energy spectra. Chaos usually manifests itself by level repulsion, while integrable systems show level clustering [33]. Type I research is not interested in exponential instabilities. Therefore, M. V. Berry suggested calling this type of research "quantum chaology" [34]. Since type I research investigates the quantized versions of classically chaotic systems, an even better name is "quantized chaos".

There is, however, a class of systems that show exponential sensitivity and complexity on the quantum mechanical level. Such systems were first discussed in the context of laser physics [35]. I call them Type II systems. Type II systems are quantum systems that are coupled to at least one classical degree of freedom. In the laser systems the classical degree of freedom is the radiation field (treated in the classical approximation). Type II quantum systems arise quite naturally in many fields of physics, in fact whenever a wave system is strongly coupled to a moving boundary [36]. In atomic physics the Born-Oppenheimer approximation provides a natural source of Type II quantum chaotic systems [37].

The last type of quantum chaotic systems are Type III systems. They are fully quantized and fully chaotic. It is possible that quasi periodically driven systems [38, 39] or systems defined on a quasi periodic spatial grid [40] may provide examples of Type III systems. Type III research, however, is still in its infancy. No truly convincing example of a Type III system was every presented.

Type I quantum chaos for the two-ion Paul trap was investigated in [41]. As long as the reaction of trapped ions on the trapping field can be neglected, Paul, Penning and Kingdon traps will not show Type II quantum chaos. The micro maser [42] is a more promising candidate for Type II quantum chaos. Type III quantum chaos can be investigated in a two-ion Paul trap driven at two different rf frequencies simultaneously.

5. Chaos and order in the Paul trap

While the single-ion Paul trap does not offer any chaos neither on the classical nor on the quantum levels, loading the Paul trap with two or more ions immediately provides a gateway to chaos. Chaotic states in the Paul trap can be identified with "clouds" of ions moving on irregular paths, whereas the regular states are the ordered "crystal" structures found to exist in a Paul trap [8, 13, 14].

The occurrence of chaos in the Paul trap provides a physical explanation for the phenomenon of "rf-heating" [16, 43]. Suppose that there are a few ions in a Paul trap, and that they are in a choatic state. Since chaos is dynamically induced disorder with no periodicity, the Fourier transform of the motion of the ions will not correspond to a picket fence of discrete frequencies, as appropriate for periodic, or quasi periodic motion, the Fourier transform will be continuous. This means that the driving frequency of the trap is contained in the frequency spectrum of a cloud and can therefore pump energy into it. This results in a net increase of kinetic energy of the ions and explains the occurrence of rf-heating in the Paul trap.

Numerical simulations of ion crystallization experiments [15, 16] showed that even in the absence of a cooling mechanism ion crystals, once formed, do not melt, even in the presence of the rf-driving field. But how is this possible? Doesn't the Paul trap show "rf-heating"? The answer is the following. So far we proved the existence of rf-heating only for ion clouds, i.e., ions in a chaotic state of motion. The motion in a crystalline configuration, however, is perfectly regular. The natural normal modes of the crystal which show up in the Fourier transform of a slightly perturbed ion crystal will not normally coincide with the rf driving frequency. Therefore, no energy transfer can occur and ion crystals don't heat.

The observed non-heating of ion crystals in a Paul trap may find a useful application in the diagnostics of the crystallized state of a cooled beam in an ion storage ring [44]. One can of course implement complicated Bragg-scattering schemes with lasers or electron beams in order to decide whether crystallization has occurred in a storage ring. Here I propose a much simpler criterion. It consists of three stages and only a Schottky pick-up is necessary to decide whether a storage ring contains a crystallized beam or not. The procedure is the following. (i) No beam cooling is switched on, the beam exhibits a Schottky noise spectrum characterized by a profile "A". (ii) The beam cooling devices are switched on. The Schottky noise settles into a new profile "B". (iii) In order to decide whether signal B corresponds to a crystalline phase, the beam cooling devices are switched off again for a certain time interval Δt which is much longer than $1000\,\mathrm{K}/\rho$, say, where ρ is a typical heating rate of the beam. After Δt has passed, the Schottky noise is checked again while the beam cooling devices are still switched off. If the noise is back to profile A, the beam resulting from stage (ii) was not crystallized. If the noise spectrum remains at B, the beam is crystallized.

One can go even one step further and define crystallization according to the criterion of the absence of heating. This criterion can be applied to both, traps and particle beams.

Many other nonlinear effects were discovered in the Paul trap including a new deterministic melting regime [11], but the chaos scenario according to which crystals in the Paul trap melt are still under investigation. A much simpler chaos scenario, in fact a scenario strongly reminiscent of the Feigenbaum scenario [31] discussed in Section 3 is displayed by the dynamic Kingdon trap. Chaos in the Kingdon trap is the subject of the next section.

6. The dynamic Kingdon Trap: Period doubling route to chaos

Imagine a straight section of charged wire. An oppositely charged ion with some initial velocity directed roughly toward the wire, but such that it will miss, will (apart from radiation losses) orbit the wire for all time and thus be trapped. This trap design is known as the static Kingdon trap [45].

The static Kingdon trap can be turned into a dynamic Kingdon trap by arranging for an ac charge on the wire in addition to the dc charge. It is known [7] that ions in an inhomogeneous ac field experience a force that is directed toward the low field regions. Thus, if the ion carries a positive charge, say, and the wire carries a negative charge, the ac defocusing field of the trap can counter balance the dc attracting field and lead to stable trapping of the ion in the effective potential minimum of both forces.

At first glance the trap contains two control parameters: the magnitudes of the ac and the dc charge, but by chosing an appropriate length scale, the number of control parameters can be reduced to one. This case, then, is quite analogous to the logistic mapping, which also contains only one control parameter. The analogy carries even further. Both the logistic mapping and the dynamic Kingdon trap display a period doubling route to chaos [17, 31]. This is the first time that I know of, that the Feigenbaum scenario appeared in a dynamic ion trap.

The period doubling scenario in the dynamic Kingdon trap is exhibited in the following way. It can be shown [17] that the equation of motion of an ion in the combined static and dynamic field of the wire is given by

$$\ddot{r} = [-1 + 2q \cos(2t)]\,\frac{1}{r} - \gamma\dot{r}, \tag{6}$$

where a small damping term $-\gamma\dot{r}$ was added to simulate laser cooling. In order to plot an r^* *vs.* q diagram in analogy to the x^* *vs.* q diagram for the logistic mapping, eq. (6) was integrated numerically for $\gamma = 10^{-4}$ for a dense grid of q values. For a given q value, the equation of motion (6) was integrated until all transients had died away and the ion settled into a stationary pattern of motion. Then, 16 subsequent positions r_j, $j = 1, 2, \ldots, 16$ of the ion at $t_j =$

0 mod π were plotted in Fig. 2 for 8000 values of q in the interval [2.916, 3.2]. Three period doubling bifurcations at $q_1 \approx 3.12$, $q_2 \approx 2.94$ and $q_3 \approx 2.917$ can be identified in Fig. 2. The maximal splittings d_1 and d_2 of the pitch forks are also shown.

On the basis of the data displayed in Fig. 2 it is not yet possible to decide whether the dynamic Kingdon trap really follows a period doubling scenario. Many more bifurcation points have to be calculated in order to approach the asymptotic behavior. Nevertheless, $\delta = 7.8$ computed from the bifurcation points shown in Fig. 2, is reasonably close to the Feigenbaum number $\delta = 8.72$, which should apply in the case of weak damping [46].

7. Summary

In this lecture I discussed some elementary aspects of chaos in general and chaos in dynamic ion traps in particular. It was shown that chaos is an important factor in the dynamics of stored ions. It is possible that some of the non-linear physics discovered in ion traps is applicable to the physics of crystallized beams and leads to new ideas in their generation and control. A first step in this direction is the proposed diagnostic procedure which consists in looking for the absence of heating as a criterion for beam crystallization.

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