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Nonlinear analysis of perturbed ion traps

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Abstract

This paper presents an analytical study of a perturbed ion trap. Various techniques are combined in order to extract information about the evolution of the system. The problem is modelled by an axially–symmetric–three–degree–of–freedom Hamiltonian. Normalization plus reduction lead to an integrable system whose flow is analyzed. Finally a qualitative relationship between the flow associated to the integrable system and the one attached to the original Hamiltonian is established. For this purpose we use estimations of the error in the normalization, Poincaré surfaces of section and KAM theory.

Key words and expressions: Hamiltonian, perturbation, trap, normalization, reduction, bifurcation.

AMS (MOS) Subject Classification: 37J40, 37J15, 37J20, 70K65.

1 Introduction

Since the beginning of last century, the effect of the application of external fields to atoms has played a crucial role in the development of atomic physics. In particular, the application of static electric and magnetic fields to create trapping phenomena is a remarkable feature. When the trapped particle is an ion, lab experiments are used to perform very precise spectroscopic measurements and to construct accurate atomic clocks. In this paper we focus on one of these experiments: the Penning trap [7, 5].

Briefly described, the Penning trap represents a three–dimensional trapping of a charge or ion due to an axially–symmetric ("*perfect*") quadrupole electric field plus a static magnetic field. The perfect quadrupole electric potential is achieved by means of a set of

three electrodes. One of the electrodes, called the ring, is shaped like the inner surface of a toroid. The other two are like hemispheres placed above and below the ring. In this arrangement, the quadrupole potential acts as a trap only in the direction of the axis between the hemispheres (we call this axis z), while the motion in the radial plane (Oxy plane) is unstable. The presence of the magnetic field along the z axis provides the complete trapping and the motion of the ion remains harmonic.

In the above ideal configuration, the Penning trap is modelled by means of an unperturbed three–dimensional harmonic oscillator with two equal frequencies [7]. However, electrostatic field perturbations may arise from imperfections in the physical design of the electrodes, as well as from misalignments in the experimental setup, see for instance Ref. [5]. We can separate these perturbations into harmonic and anharmonic perturbations. In particular, it is the second group the most interesting one because it leads to nonlinear motion. In this paper we only consider axially–symmetric perturbations of the three–dimensional Penning trap. In particular, we will treat the *sextupolar* perturbation. In this way the third component of the angular momentum vector is an exact integral of the whole perturbed system.

Hence, the model is ideal to be considered from an analytical point of view within the framework of perturbation theory. Our goal is to perform a qualitative analysis of the effect caused by the imperfections on the Penning trap.

2 Formulation of the Problem

In this paper we present the model under study skipping the procedure to obtain the formulation from the physical system. For that, the reader is referred to [6]. We consider the Hamiltonian $\mathcal{H}$ in Cartesian coordinates x, y, z and conjugate momenta p_x, p_y, p_z:

$$\mathcal{H} = \frac{1}{2\,m}\,(p_x^2 + p_y^2 + p_z^2) + \frac{m}{2}\,w^2\,(x^2 + y^2) + \frac{m}{2}\,w_z^2\,z^2 + a_3\,z\,(2\,z^2 - 3\,x^2 - 3\,y^2). \qquad (1)$$

Quadratic terms in $\mathcal{H}$ stand for the Hamiltonian corresponding to a single ion of mass m trapped in a *perfect* Penning trap, where w_z is the frequency induced by the quadrupole electric field and $w > 0$ represents the trapping condition. Cubic terms in $\mathcal{H}$ stand for the sextupolar perturbation. Thus, a_3 is considered as the sextupole parameter.

By assuming a_3 to be small, we can consider the system defined by Hamiltonian (1) as a weakly perturbed $w{:}w{:}w_z$ harmonic oscillator. In the particular case $w_z = w$ (the isotropic case), Hamiltonian (1) corresponds to the Hénon and Heiles system in three dimensions [3]. When $w_z \neq w$, in order to still consider (1) as a weakly perturbed isotropic oscillator, we will assume $w_z \approx w$. This allows us to define a small detuning parameter $|\delta| \ll 1$ in such a way that it is possible to split $w_z^2 = w^2 + \delta\,w^2$. Therefore,

Hamiltonian (1) becomes

$$\begin{aligned}
\mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_1, \\
\mathcal{H}_0 &= \frac{1}{2\,m}\,(p_x^2 + p_y^2 + p_z^2) + \frac{m}{2}\,w^2\,(x^2 + y^2 + z^2), \\
\mathcal{H}_1 &= \frac{m}{2}\,\delta\,w^2\,z^2 + a_3\,z\,(2\,z^2 - 3\,x^2 - 3\,y^2),
\end{aligned} \tag{2}$$

where $\mathcal{H}_1$ is the perturbation to $\mathcal{H}_0$.

3 Normalization and Reduction

Our aim in this section is to simplify Hamiltonian $\mathcal{H}$. Here we sketch the ideas for the procedure and present the results. For details, see [6]. First we perform an asymptotic transformation up to second order of approximation. After fixing the value of the energy we will reach a two–degree–of–freedom system. The transformation is constructed in such a way that we average the original system over one of the angles. Indeed, the high–order averaging procedure can be interpreted as a normalization technique since the "elimination" of an angle variable is completely equivalent to the construction of a formal integral, see for instance [8]. At this point we want to emphasize that this type of transformations are, in general, divergent. However, one can still build approximations to the original problem (e.g. normalized or averaged Hamilton functions) good enough to be useful for analytical purposes. This must be accompanied by an estimate of the error made after truncation of the high–order terms.

The normalization procedure is carried out by means of Lie transformations following the Lie–Deprit method, see Ref. [2]. We use nodal–Lissajous variables (ℓ, g, ν, L, G, N), a set of action–angle variables which describe particularly well axially–symmetric perturbations of oscillators in 1–1–1 resonance, see Refs. [3].

In this case, we compute the averaged Hamiltonian up to second order because at this order we have a finite number of equilibria in the reduced phase space, as we will see in next section. Thence, higher orders in the normalized system do not alter the qualitative behaviour of the reduced system.

As we have pointed out before, the presence of the axial symmetry, not only in the perturbation, but also in the unperturbed part of $\mathcal{H}$, allows the system to be reduced again. In contrast with the first reduction, this second one is singular, the twice–reduced space (from now on we call it $\mathcal{T}$) is not a smooth surface. Depending on the value of the z–component of the angular momentum N the shape of this phase space is either a double–pinched sphere (lemon), when $N = 0$, or a single–pinched one (balloon), if $N \neq 0$, Ref. [1].

Fixing values for N and L, the double–reduced space is two–dimensional and is described by three linearly independent invariants $(\tau_1', \tau_2', \tau_3')$ constrained by: $|N'| \leq \tau_2' \leq 1$ with $N' = N/L$ and

$$\tau_1'^2 + \tau_3'^2 = (1 - \tau_2')^2 \, (\tau_2'^2 - N'^2). \tag{3}$$

Each point in the double–reduced phase space defined by (3) corresponds to a family of perturbed ellipses in the original phase space.

Once we have applied the two reductions described above to Hamiltonian (2) we obtain:

$$\mathcal{K}_d = \alpha \, \left(\gamma \, \tau_2' + 16 \, \tau_1' + 41 \, \tau_2'^2 - 56 \, \tau_2' \right), \tag{4}$$

where $\alpha = 3 \, a_3^2 \, L / w^5$, which indicates the ratio between the frequency of the unperturbed oscillator and the frequency induced by the sextupolar term and $\gamma = \delta \, (4 - \delta)/(2 \, \alpha)$, which in fact accounts for the relative influence between the detuning and the sextupolar perturbation. Hence, Hamiltonian (4) contains the relevant dynamical information of system $\mathcal{H}$, depending on the two parameters γ and N' (which appears in Eq. (3)).

4 Phase Flow in the Reduced System

Taking into account the Poisson brackets between the variables [6] we derive the equations of the motion

$$\begin{aligned}
\dot{\tau}_1 &= \{ \, \tau_1 \, , \, \mathcal{K}_d \, \} = -\frac{2\alpha}{L} \, (82\tau_2 - 56 + \gamma) \, \tau_3, \\
\dot{\tau}_2 &= \{ \, \tau_2 \, , \, \mathcal{K}_d \, \} = \frac{32\alpha}{L} \, \tau_3, \\
\dot{\tau}_3 &= \{ \, \tau_3 \, , \, \mathcal{K}_d \, \} = \frac{2\alpha}{L} \, \left[16N^2(1 - \tau_2) + (82\tau_2 - 56 + \gamma)\tau_1 + 16(1 - 3\tau_2 + 2\tau_2^2)\tau_2 \right].
\end{aligned} \tag{5}$$

Note that we have dropped the primes for the sake of simplicity.

The equilibria of the system are the local extrema of $\mathcal{K}_d$ on the semialgebraic variety (3). They are the roots of the system formed by the right hand members of (5) equated to 0 together with the constraint (3).

We give here some general information about this system. For details on its discussion, see [6]. From the second equation of (5), it follows that the equilibrium points are located on the plane $\tau_3 = 0$. There always exists one equilibrium point, namely $(0, 1, 0)$. The maximum number of equilibria is four, whereas the minimum is two. The change in the number of equilibria owes to two different reasons. The first one is that one of the roots enters or leaves the interval taking the extreme values $|N|$ or 1, whereas the second is that two or more roots explode from a multiple root. According to these changes, the parameter plane (γ, N) is divided into regions R_1, R_2, R_3, R_4 by the bifurcation lines A, B and the segment C (see Fig. 1). The analytic expressions for the bifurcations can be seen in [6].

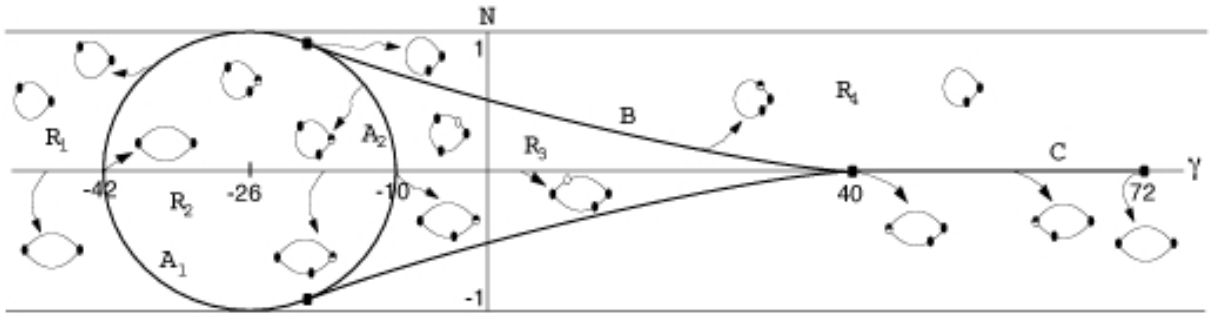

Figure 1: Bifurcation diagram and meridian sections $\tau_3 = 0$ of balloons and lemons. Stable points (index=1) are characterized by a black circle while unstable points with index -1 are by a white one and the ones with index 0 are represented by a black–white circle.

In order to study the stability of the equilibria appearing in all regions of the parametric plane, we combine two techniques. On the one hand, for the equilibria appearing in the regular points of the balloons and lemons we use the standard method of Lagrange multipliers; on the other hand, the stability of the singular points can be deduced from the Index Theorem once the stability behaviour of the regular equilibria has been established. See the results in Fig. 1 and details in [6].

With respect to the type of bifurcations that occur we detect the following four:

Line B corresponds to a *saddle-centre* bifurcation. Whereas line A_1 is a *Hamiltonian flip* bifurcation of *subtle* type, A_2 is a *Hamiltonian flip* bifurcation of *murder* type. A *Hamiltonian Hopf* bifurcation occurs when the value $\gamma = 72$ is reached while moving along $N = 0$. Finally, the segment C corresponds also to a bifurcation. For a detailed description of these bifurcations see [6] and references therein.

A complementary information about the dynamics of the system is obtained from the phase flow evolution. For details on how to perform the calculations involved to determine the phase flow and some visualizations, see [6].

5 Connection to the Original System

5.1 Estimate of the error of the Lie transformation

The (formal and symplectic) change of variables applied in Section 3 can be used to calculate an upper bound of the error committed in the truncation of the Lie transformation approach.

Given $\mathbf{x} = (x, y, z, p_x, p_y, p_z)$ and $\mathbf{x}' = (x', y', z', p'_x, p'_y, p'_z)$ we calculate the change $\mathbf{x}' = \mathbf{X}'(\mathbf{x}; \varepsilon)$. Note that $\mathbf{X}'$ gives explicit expressions of the new (transformed) variables $\mathbf{x}'$ in terms of the old (original) variables $\mathbf{x}$. Furthermore, we compute $\mathbf{x} = \mathbf{X}(\mathbf{x}'; \varepsilon)$

obtaining expressions of the old variables $\mathbf{x}$ as functions of the new variables $\mathbf{x}'$. At this step we have to mention that both $\mathbf{X}$ and $\mathbf{X}'$ are constructed by means of the generating function using the formulae given in [2]. Moreover both changes $\mathbf{X}$ and $\mathbf{X}'$ are built up to second order in the small parameter ε.

We can compose $\mathbf{X}$ with $\mathbf{X}'$ and compute explicitly the vector field $\mathbf{X}(\mathbf{X}'(\mathbf{x};\varepsilon);\varepsilon)$, which must be indeed a second–order approximation to $\mathbf{x}$. Hence we arrive at

$$\|\mathbf{x} - \mathbf{X}(\mathbf{X}'(\mathbf{x};\varepsilon);\varepsilon)\| = \varepsilon^3$$

$\mathrm{E}(\mathbf{x})+\mathrm{O}(\varepsilon^4), (6)$where $\|\cdot\|$ denotes the Euclidean norm in $\mathbf{R}^6$ and $E(\mathbf{x})$ is the global error term, which is obtained explicitly and depends on the three coordinates, their three conjugate moments and the two significant parameters of the problem, say γ and α or, going back to the original Hamiltonian, the parameters a_3 and δ. Note that for this particular problem the parameter ε can be set equal to 1 as the real small parameters are inside the function E.

Now we have to bound the function E. Assuming that a_3 and δ satisfy $|a_3| \leq 5 \times 10^{-2}$ and $|\delta| \leq 3 \times 10^{-1}$, we have checked numerically that $|E(\mathbf{x})| \leq 5 \times 10^{-3}$ provided that $\|\mathbf{x}\| \leq 1.25$. This calculation shows the efficiency of the analytical approach, valid in a neighbourhood of the origin of $\mathbf{R}^6$. Note that this result is in agreement with the values obtained after truncation of the Lie transformation at second order since $|E(\mathbf{x})|$ is of the order of $\mathcal{O}(\varepsilon^3)$.

5.2 Poincaré surfaces of section

We can validate the estimation of the latter subsection by the analysis of the original Hamiltonian by means of the technique of Poincaré surfaces of section (PSS). In fact, we have established a correspondence between the fixed points in the PSS and the relative equilibria. For pictures and details see [6].

In this way, we find out a direct connection between periodic orbits in the original system and critical points in the reduced phase space. Besides this remarkable connection we also observe the same qualitative evolution as γ varies. In fact, both the original and the twice–reduced system $\mathcal{T}$ undergo the same sequence of bifurcations. Concretely, the Hamiltonian flip bifurcation in balloons and lemons turns to be a pitchfork bifurcation in the surfaces of section. This is due to the 2:1 covering of the twice–reduced phase space (see Ref. [4]). Moreover, the Hamiltonian Hopf bifurcation remains the same in both the surfaces of section and the lemons and balloons.

5.3 Dynamics of the full system: KAM theory

Since the normalized Hamiltonian $\mathcal{K}_d$ has been obtained after two reduction procedures (the second–order normalization followed by the exact axial–symmetry reduction), we

have to attach a 2D torus to any point of the reduced phase space $\mathcal{T}$. More concretely, if $|N| < G < L$, i.e. when the nodal–Lissajous variables are well defined, the 2D tori are parameterized by the angles ℓ and ν. (However, in case of equatorial or circular trajectories it is still possible to define other action–angle variables and perform the reconstruction of the invariant manifolds similarly.)

In particular one should speak of families of 2D tori depending on the parameters L and N. This means that equilibrium points on the balloons and on the lemons must be understood as invariant 2D tori in $\mathbf{R}^6$. Moreover they enjoy the same type of stability whenever all the eigenvalues of the linearization of each equilibrium have non–null real part. One can even compute explicit formulae of the (truncated) invariant 2D tori using the direct change of the Lie transformation.

In those equilibria of $\mathcal{T}$ where the linearization gives eigenvalues with null real part, a specific analysis should be performed. Nevertheless, in this problem such situations occur only on the bifurcation curves A, B and the point $(\gamma, N) = (72, 0)$, which correspond, respectively, to Hamiltonian flip, saddle–centre and Hamiltonian Hopf bifurcations (note that this has been numerically verified in the latter subsection using the surfaces of section). For the analysis of these cases we refer to the papers [4] and [1] where these bifurcations also occurs. Hence, all the details about the reconstruction process can be followed in those papers. The bifurcations of relative equilibria are translated into bifurcations of 2D invariant tori or quasiperiodic orbits. Moreover the persistence of these bifurcations is guaranteed by the estimate derived in Subsection 5.1.

5.4 Physical interpretation

In this paper we have shown that, for a fixed value of N, the dynamics is governed by the parameter which indicates the relative influence between the detunig δ and the sextupolar imperfection a_3. If we focus on the polar case $N = 0$, which is the easiest to be achieved experimentally, when γ goes from 0 ($\delta = 0$) to $\gamma > 72$ or to $\gamma < -42$, in both cases the phase space evolve to rotations around two stable equilibria through several bifurcations. It is worth noting that this situation is equivalent to the one where the sextupolar perturbation is not present ($a_3 = 0$). As for $a_3 = 0$ the system is integrable the nonlinear character of the problem is provided by the sextupolar term. Thus, we can conclude that the presence of the detuning attenuates the nonlinear effects caused by the sextupolar perturbation. Taking into account that the value of the detuning can be controlled, this perturbative study can serve to decide which detuning added to the sextupolar perturbations would suppress the chaotic behaviour induced by the sextupolar term when one treats the complete problem.

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