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# Chaos and randomness in a classical bistable system coupled to a finite heat bath

Santiago Peña Martínez



Universidad Nacional de Colombia

This dissertation is submitted on July, 2020 for the degree of Bachelor in Physics



## DECLARATION

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This dissertation is the result of my own work and includes nothing which is the outcome of work done in collaboration except as declared in the Preface and specified in the text. It is not substantially the same as any that I have submitted, or am concurrently submitting, for a degree or diploma or other qualification at the Universidad Nacional de Colombia or any other University or similar institution except as declared in the Preface and specified in the text. I further state that no substantial part of my dissertation has already been submitted, or is being concurrently submitted, for any such degree, diploma or other qualification at the Universidad Nacional de Colombia or any other University or similar institution except as declared in the Preface and specified in the text.

Santiago Peña Martínez  
Month, Year



## ABSTRACT

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### **Chaos and randomness in a classical bistable system coupled to a finite heat bath**

*Santiago Peña Martínez*

In this work we study a double well potential coupled to a finite heat bath consisting of  $N$  harmonic oscillators. For  $N = 1$ , the system will oscillate in an irregular manner between the symmetric minima involving chaotic properties. As we increase  $N$  to values  $> 1$ , the system will approach a bistable behaviour, according to the microscopic theory of dissipation. In particular, the system will irreversibly fall into one of the wells, imitating the result of a measurement of two alternative states. Which well it chooses will depend on the initial state of the system and the heat bath, meaning that the information encoded in the microscopic initial conditions is amplified and recorded in the final state, as in a measurement.

Keywords: Chaos, Dissipation, Measurement.



## ACKNOWLEDGEMENTS

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My acknowledgements ...





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## INTRODUCTION REVISARLA

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The concept of measurement in quantum mechanics has been a fuzzy concept ever since the origins of the quantum theory because there is not a precise description of what happens when physicists say that the wave function “collapses”. This lack of description of the moment of the collapse and the inability to observe this phenomenon directly lead to different interpretations of quantum mechanics (CITAR Decoherence, the measurement problem, and interpretations of quantummechanics- SCHLOSSHAUER). In this work we do not intent to solve this problem in the quantum mechanics frame but we will show an approach to study this problem by looking at a classical analogue of the spin and describing in classical terms the effect that an environment has in the outcome of what we will call a measurement.

When considering the effects of an environment enclosing a system of interest, most of the times you arrive to a problem that is difficult model and solve. Generally when trying to model an environment it consists of a large number of degrees of freedom, this leads to adopting tools such as Langevin dynamics and statistical methods to try to solve this problem, this makes microscopic effects on the system have a role in the macroscopic dynamics.

Some of the first approaches to model environments in statistical physics where made to model properly the Brownian motion (CITE CITAR R. Brow, Philosophical Magazine N. S., 4, 161, 1828 A. Einstein, Ann. der Phys., 17, 549, 1905 R. Kubo, Science, 233, 330, 1986.). The original Langevin equation (CITAR CITE Langevin, P. (1908). ”Sur la théorie du mouvement brownien ) was used to describe Brownian motion, this approach consists on describing the system in a way that all of the effects of the environment are contained in a time-dependent force term and a velocity dependent friction of damping term. The force term behaves as a stochastic process representing the “randomness” of the environment affecting the central system. This method is widely used to study the properties of the central system without

going into the details of the environment. It is important to state here that the environment is and will be considered as a heat bath in the thermodynamic sense, where the central system can exchange energy back and forth in time until thermal equilibrium is reached.

# BACKGROUND

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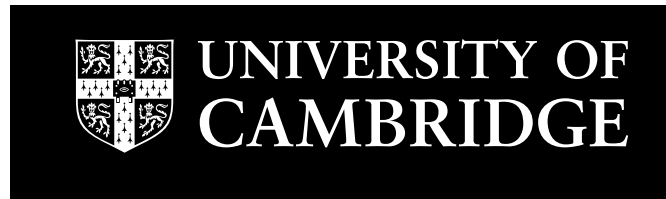


Figura 2.1: An inverted black and white version of the Cambridge University logo.

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# HAMILTONIAN SYSTEMS AND SYMPLECTIC STRUCTURE- OTT Y JOAO

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In this chapter we are going to introduce some important concepts regarding dynamical systems and how they relate to hamiltonian systems and its geometric structure. Also we describe the theory involving the numerical integration of differential equations conserving the symplectic structure. These descriptions are made following Ref. [?] and Ref. FALTA CITA DE INTEGRADORES NUMERICOS SIMPLECTICOS

### 3.1. Dynamical systems- OTT Y JOAO

Generally speaking, a dynamical system may be defined as set of deterministic mathematical equations whose solution shows how the system evolves in time. Time may be taken as a continuous or a discrete variable. An example of a dynamical system with time as a parameter varying in a continuous way is a system of  $n$  first order, autonomous, ordinary differential equations,

$$\begin{aligned}\frac{dx^{(1)}}{dt} &= F_1(x^{(1)}, x^{(2)}, \dots, x^{(n)}), \\ \frac{dx^{(2)}}{dt} &= F_2(x^{(1)}, x^{(2)}, \dots, x^{(n)}), \\ &\vdots \\ \frac{dx^{(n)}}{dt} &= F_n(x^{(1)}, x^{(2)}, \dots, x^{(n)}),\end{aligned}\tag{3.1}$$

this set of equations may be written as a compact equation using the vector form of equations

$$\frac{d\vec{x}(t)}{dt} = \vec{F}[\vec{x}(t)],$$

where  $\vec{x}$  is an  $n$  dimensional vector that represents the state of the system at a given time  $t$  and  $\vec{F}$  is a function of the variable  $\vec{x}$ . This set of equations represent a dynamical system, for an initial state given by  $\vec{x}(0)$ , we may be able in principle to solve the set of equations and obtain the state  $\vec{x}(t)$  of the system for any given  $t > 0$ . The figure FIGURA QUE NO HE HECHO shows the points followed as the system evolves in time for the case of  $n = 3$ . The space  $(x^{(1)}, x^{(2)}, x^{(3)})$  in the figure is more known as the phase space, and the path in the phase space is referred as orbit or trajectory. In the case of dynamical systems of continuous time, it is common to refer to these orbits as a flow.

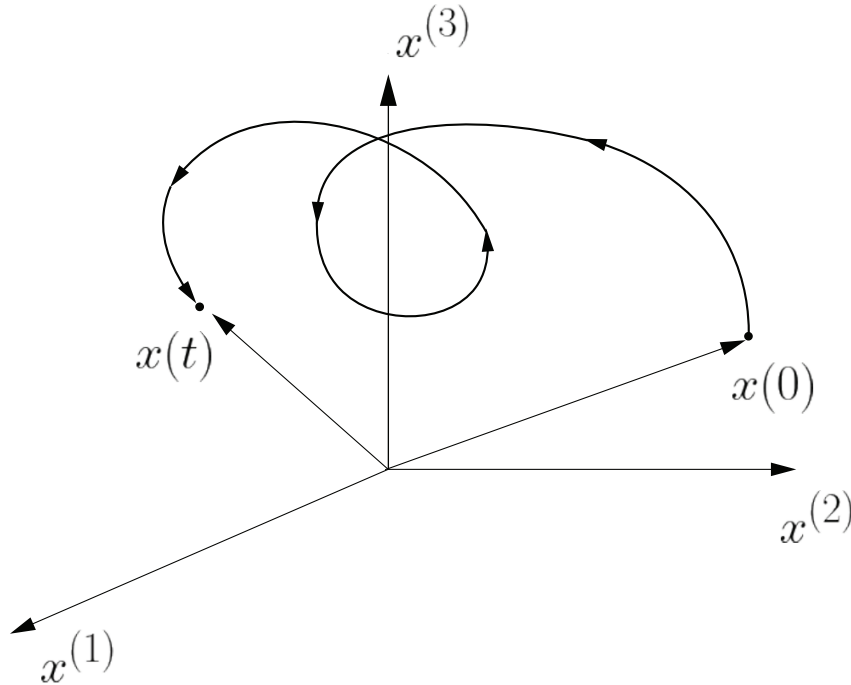


Figura 3.1: Orbit in three dimensional phase space

For the case of discrete systems, time is represented as integer values ( $t = 1, 2, 3, \dots$ ). An example of a dynamical system with discrete time is a map, which can be written as vector form as

$$\vec{x}_{t+1} = \vec{M}(\vec{x}_t) \quad (3.3)$$

where  $\vec{x}_t$  is an  $n$ -dimensional vector  $\vec{x}_t = (x_t^1, x_t^2, \dots, x_t^n)$  and  $\vec{M}$  a function of  $\vec{x}_t$ . Given an initial state  $\vec{x}_0$ , it is possible to obtain the state at time  $t = 1$  by  $\vec{x}_1 = \vec{M}(\vec{x}_0)$ . Having determined  $\vec{x}_1$  it will be possible to determine the state at time  $t = 2$  by  $\vec{x}_2 = \vec{M}(\vec{x}_1)$  and so on. Thus, given an initial condition  $\vec{x}_0$  we generate a trajectory of the discrete time system:  $\vec{x}_0, \vec{x}_1, \vec{x}_2, \dots$

A dynamical system that posses continuos time evolution may be reduced to a discrete time system by using the technique called Poincaré Surface Section. We consider a set of  $n$  first order, autonomous, ordinary differential equations ??, a Poincaré map represents a reduction of the flow in the  $n$ -dimensional space to a map of dimension  $n - 1$ . To illustrate this, an example with  $n = 3$  is given:

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Fig (NUMERO DE LA FIGURA) is a Poincaré section on a two dimensional plane  $S$  on  $x^3 = constant$ . The points A and B represent the successive intersections of the trajectory followed by the system with the plane  $S$ , this crossing is always on the same direction. Given a point A, using Eq. (??), we can determine the position of point B, this is because A can be used as an initial condition to determine B. The same argument can be used to determine A given B as initial condition by changing the sign of time on the same equation. Thus, the Poincaré map in this illustration represents an invertible two dimensional map transforming the coordinates  $(x_n^{(1)}, x_n^{(2)})$  of the  $n$ th piercing of the surface section to the coordinates  $(x_{n+1}^{(1)}, x_{n+1}^{(2)})$  at piercing  $n + 1$ . This map can be generalized to an  $N$  dimensional flow with an  $N - 1$  dimensional invertible map.

## 3.2. Hamilton equations and Symplectic Structure- OTT Y JOAO

Hamiltonian systems are a class of dynamical systems that occur in a wide variety of circumstances. The special properties of Hamilton's equations endow these systems with attributes that differ qualitatively and fundamentally from other systems.

The dynamics of a Hamiltonian system is completely specified by a single function, the Hamiltonian,  $H(\mathbf{p}, \mathbf{q}, t)$ . The state of the system is specified by its "momentum" and "position" usually known as  $\mathbf{p}$  and  $\mathbf{q}$  respectively, both vectors with dimension  $N$ .  $N$  is also known as the number of degrees of freedom of the system. The Hamilton's equations determine the trajectory  $(\mathbf{p}(t), \mathbf{q}(t))$  the system follows in the  $2N$  dimensional phase space, these equations are given by

$$\frac{d\mathbf{p}}{dt} = -\frac{\partial H(\mathbf{p}, \mathbf{q}, t)}{\partial \mathbf{q}}, \quad (3.4)$$

$$\frac{d\mathbf{q}}{dt} = \frac{\partial H(\mathbf{p}, \mathbf{q}, t)}{\partial \mathbf{p}}. \quad (3.5)$$

In the special case that the Hamiltonian has no explicit time dependance,  $H = H(\mathbf{p}, \mathbf{q})$ , we can use Hamilton's equations to show that, as  $\mathbf{p}$  and  $\mathbf{q}$  vary with time, the value of  $H(\mathbf{p}(t), \mathbf{q}(t))$  remains constant:

$$\frac{dH}{dt} = \frac{d\mathbf{q}}{dt} \frac{\partial H(\mathbf{p}, \mathbf{q})}{\partial \mathbf{q}} + \frac{d\mathbf{p}}{dt} \frac{\partial H(\mathbf{p}, \mathbf{q})}{\partial \mathbf{p}} = \frac{\partial H(\mathbf{p}, \mathbf{q})}{\partial \mathbf{p}} \frac{\partial H(\mathbf{p}, \mathbf{q})}{\partial \mathbf{q}} - \frac{\partial H(\mathbf{p}, \mathbf{q})}{\partial \mathbf{q}} \frac{\partial H(\mathbf{p}, \mathbf{q})}{\partial \mathbf{p}} = 0$$

Thus identifying the value of the Hamiltonian with the energy  $E$  of the system, we see that the energy is conserved in the case of time independent systems,  $E = H(\mathbf{p}, \mathbf{q}) = \text{constant}[?]$ .

Another particularity of Hamilton equations and Hamiltonian systems is that we can write Eqs. (3.4, 3.5) in matrix form as

$$\frac{d\tilde{\mathbf{x}}}{dt} = \mathbf{F}(\tilde{\mathbf{x}}, t), \quad (3.6)$$

by taking  $\tilde{\mathbf{x}}$  to be the  $2N$  dimensional vector

$$\tilde{\mathbf{x}} = \begin{pmatrix} \mathbf{p} \\ \mathbf{q} \end{pmatrix}, \quad (3.7)$$

and by taking  $\mathbf{F}(\tilde{\mathbf{x}}, t)$  to be

$$\mathbf{F}(\tilde{\mathbf{x}}, t) = \mathbf{S}_N \cdot \frac{\partial H}{\partial \tilde{\mathbf{x}}}, \quad (3.8)$$

where  $\mathbf{S}_N$  is the so called symplectic matrix given by

$$\mathbf{S}_N = \begin{bmatrix} \mathbf{O}_N & -\mathbf{I}_N \\ \mathbf{I}_N & \mathbf{O}_N \end{bmatrix} \quad (3.9)$$

where  $\mathbf{I}_N$  is the  $N$  dimensional identity matrix,  $\mathbf{O}_N$  is the  $N \times N$  matrix of zeros, and

$$\frac{\partial H}{\partial \tilde{\mathbf{x}}} = \begin{bmatrix} \partial H / \partial \mathbf{p} \\ \partial H / \partial \mathbf{q} \end{bmatrix} \quad (3.10)$$

From this we see how restricted the class of Hamiltonian systems is. In particular, a general system of the form (3.6) requires the specification of all the components of the vector function  $\mathbf{F}(\tilde{\mathbf{x}}, t)$ , while by (3.8), if the system is Hamiltonian, it is specified by a single scalar function of  $\mathbf{p}$ ,  $\mathbf{q}$  and  $t$  (the Hamiltonian).

One of the basic properties of Hamilton's equations is that they preserve  $2N$  dimensional volumes in the phase space. This follows by taking the divergence of  $\mathbf{F}(\tilde{\mathbf{x}})$  in Eq. (3.6), which gives

$$\nabla \cdot \mathbf{F} = \frac{\partial}{\partial \tilde{\mathbf{x}}} \cdot \mathbf{F} = \frac{\partial}{\partial \mathbf{p}} \cdot \left( -\frac{\partial H}{\partial \mathbf{q}} \right) + \frac{\partial}{\partial \mathbf{q}} \cdot \left( \frac{\partial H}{\partial \mathbf{p}} \right) = 0 \quad (3.11)$$

Thus, if we consider an initial closed surface  $S_0$  in the  $2N$  dimensional phase space and evolve each point on the surface forward with time, we obtain at each instant of time  $t$  a new closed surface  $S_t$  which contains within it precisely the same  $2N$  dimensional volume as does  $S_0$ . This follows from

$$\frac{d}{dt} \int_{S_t} d^{2N} \tilde{\mathbf{x}} = \oint_{S_t} \frac{d\tilde{\mathbf{x}}}{dt} \cdot d\mathbf{S} = \oint_{S_t} \mathbf{F} \cdot d\mathbf{S} = \int_{S_t} \frac{\partial}{\partial \tilde{\mathbf{x}}} \cdot d^{2N} \tilde{\mathbf{x}} = 0, \quad (3.12)$$

where  $\int_{S_t} \dots$  denotes integration over the volume enclosed by  $S_t$ ,  $\oint_{S_t} \dots$  denotes a surface integral over the closed surface  $S_t$ , and the third equality is from the divergence theorem [? ]. As a consequence of this result, Hamiltonian systems do not have attractors in the usual sense. This incompressibility of phase space volumes for Hamiltonian systems is called Liouville's

theorem [?] CITAR AL GOLDSTEIN.

Perhaps the most important basic structural property of Hamilton's equations is that they are symplectic [? ]:

$$\frac{d\tilde{\mathbf{x}}}{dt} = \mathbf{S}_N \cdot \frac{\partial H}{\partial \tilde{\mathbf{x}}}. \quad (3.13)$$

That is, if we consider three orbits that are infinitesimally displaced from each other,  $(\mathbf{p}(t), \mathbf{q}(t))$ ,  $(\mathbf{p}(t) + \delta\mathbf{p}(t), \mathbf{q}(t) + \delta\mathbf{q}(t))$  and  $(\mathbf{p}(t) + \delta\mathbf{p}'(t), \mathbf{q}(t) + \delta\mathbf{q}'(t))$ , where  $\delta\mathbf{p}$ ,  $\delta\mathbf{q}$ ,  $\delta\mathbf{p}'$  and  $\delta\mathbf{q}'$  are infinitesimal  $N$  vectors, then the quantity,

$$\delta\mathbf{p} \cdot \delta\mathbf{q}' - \delta\mathbf{q} \cdot \delta\mathbf{p}', \quad (3.14)$$

which we call the differential symplectic area, is independent of time,

$$\frac{d}{dt}(\delta\mathbf{p} \cdot \delta\mathbf{q}' - \delta\mathbf{q} \cdot \delta\mathbf{p}') = 0. \quad (3.15)$$

The differential symplectic area can also be written as

$$\delta\mathbf{p} \cdot \delta\mathbf{q}' - \delta\mathbf{q} \cdot \delta\mathbf{p}' = \delta\tilde{\mathbf{x}}^\dagger \cdot \mathbf{S}_N \cdot \delta\tilde{\mathbf{x}}' \quad (3.16)$$

where  $\dagger$  denotes transpose.

To derive (3.15) we differentiate (3.16) with respect to time and use Eqs. (3.6) - (3.10):

$$\begin{aligned} \frac{d}{dt}(\delta\tilde{\mathbf{x}}^\dagger \cdot \mathbf{S}_N \cdot \delta\tilde{\mathbf{x}}') &= \frac{d\delta\tilde{\mathbf{x}}^\dagger}{dt} \cdot \mathbf{S}_N \cdot \delta\tilde{\mathbf{x}}' + \delta\tilde{\mathbf{x}}^\dagger \cdot \mathbf{S}_N \cdot \frac{d\delta\tilde{\mathbf{x}}'}{dt} \\ &= \left( \frac{\partial \mathbf{F}}{\partial \tilde{\mathbf{x}}} \cdot \delta\tilde{\mathbf{x}} \right)^\dagger \cdot \mathbf{S}_N \cdot \delta\tilde{\mathbf{x}}' + \delta\tilde{\mathbf{x}}^\dagger \cdot \mathbf{S}_N \cdot \frac{\partial \mathbf{F}}{\partial \tilde{\mathbf{x}}} \cdot \delta\tilde{\mathbf{x}}' \\ &= \delta\tilde{\mathbf{x}}^\dagger \cdot \left[ \left( \frac{\partial \mathbf{F}}{\partial \tilde{\mathbf{x}}} \right)^\dagger \cdot \mathbf{S}_N + \mathbf{S}_N \cdot \frac{\partial \mathbf{F}}{\partial \tilde{\mathbf{x}}} \right] \cdot \delta\tilde{\mathbf{x}}' \\ &= \delta\tilde{\mathbf{x}}^\dagger \cdot \left[ \left( \mathbf{S}_N \cdot \frac{\partial^2 H}{\partial \tilde{\mathbf{x}} \partial \tilde{\mathbf{x}}} \right)^\dagger \cdot \mathbf{S}_N + \mathbf{S}_N \cdot \mathbf{S}_N \cdot \frac{\partial^2 H}{\partial \tilde{\mathbf{x}} \partial \tilde{\mathbf{x}}} \right] \cdot \delta\tilde{\mathbf{x}}' \\ &= \delta\tilde{\mathbf{x}}^\dagger \cdot \left[ \left( \frac{\partial^2 H}{\partial \tilde{\mathbf{x}} \partial \tilde{\mathbf{x}}} \right)^\dagger \cdot \mathbf{S}_N^\dagger \cdot \mathbf{S}_N + \mathbf{S}_N \cdot \mathbf{S}_N \cdot \frac{\partial^2 H}{\partial \tilde{\mathbf{x}} \partial \tilde{\mathbf{x}}} \right] \cdot \delta\tilde{\mathbf{x}}' \\ &= 0, \end{aligned} \quad (3.17)$$

where we have used  $\mathbf{S}_N \cdot \mathbf{S}_N = -\mathbf{I}_{2N}$  (where  $\mathbf{I}_{2N}$  is the  $2N$  dimensional identity matrix),  $\mathbf{S}_N^\dagger = -\mathbf{S}_N$  and noted that  $\partial^2 H / \partial \tilde{\mathbf{x}} \partial \tilde{\mathbf{x}}$  is a symmetric matrix. Then the symplectic matrix  $\mathbf{S}_N$



satisfies the following conditions CITE ARNOLD ERGODIC PROBLEMS OF CLASSICAL MECHANICS :

$$\mathbf{S}_N^{-1} = \mathbf{S}_N^\dagger = -\mathbf{S}_N \quad (3.18)$$

and

$$\det(\mathbf{S}_N) = 1, \quad (3.19)$$

which can be obtained directly from Eq.(3.9).

Symplectic systems present a wide variety of properties CITE ARNOLD ERGODIC PROBLEMS OF CLASSICAL MECHANICS, but the one that is more relevant for this work, is that they conserve the volume on the  $2N$  dimensional phase space, this means that symplectic dynamical systems follow the Liouville Theorem [? ].

The fact that a Hamiltonian system conserves volume in the phase space has some consequences, we will highlight here the Poincare Recurrence Theorem CITE ZASLAVSKI HAMILTONIAN CHAOS AND FRACTIONAL DYNAMICS AND ZASLAVSKI THE PHYSICS OF CHAOS IN HAMILTONIAN SYSTEMS. When considering the movement of the system in a limited region of the phase space, which we denote as  $\Gamma$ , if we define a small area  $A$  within this region (REF FIGURA QUE NO HE HECHO), with volume  $\Gamma_A < \Gamma$ , we can obtain a set of time values  $\{t_j\}$  for which the flow crosses this region from the inside out. The time intervals

$$\tau_j = t_{j+1} - t_j; \quad j = 0, 1, 2, \dots \quad (3.20)$$

are the Poincare Cycles and  $t_j$  the Poincare Recurrence Times.

FIGURA QUE NO HE HECHO DE LA REFERENCIA DE LOS CICLOS DE POINCARÉ

Poincare proved that for a movement in a finite region of space in which the volume is preserved, the entire path would return to a previously determined region (for example  $A$  in Fig. FIGURA QUE NO HE HECHO) in a finite time and an infinite number of times. An exception occurs only if  $A$  is a zero dimension set CITE ZASLAVSKI HAMILTONIAN CHAOS AND FRACTIONAL DYNAMICS AND ZASLAVSKI THE PHYSICS OF CHAOS IN HAMILTONIAN SYSTEMS.

Thus, some general properties of Hamiltonian dynamical systems have been described. This occurred without taking into account its movement, that is, its dynamics. In the coming sections, this question starts to gain space, focusing attention on some characteristics of its dynamics, more specifically when there is the presence of regular movement, chaos or a mixture of both.

### 3.2.1. Integrability in Hamiltonian problems

As we have previously stated, the case where the Hamiltonian has no explicit time dependence,  $H = H(\mathbf{p}, \mathbf{q})$ , we have seen that Hamilton's equations imply that  $dH/dt = 0$  and the energy  $E = H(\mathbf{p}, \mathbf{q})$  is a conserved quantity. Thus, orbits with a given energy  $E$  are restricted to lie on the  $(2N - 1)$  dimensional surface  $E = H(\mathbf{p}, \mathbf{q})$ . A function  $f(\mathbf{p}, \mathbf{q})$  is said to be a constant of motion of for a system with Hamiltonian  $H$  is a constant of motion. More generally, differentiating  $f(\mathbf{p}, \mathbf{q})$  with respect to time, and assuming that there is no explicit time dependence of the Hamiltonian, we have

$$\frac{df}{dt} = \frac{d\mathbf{p}}{dt} \cdot \frac{\partial f}{\partial \mathbf{p}} + \frac{d\mathbf{q}}{dt} \cdot \frac{\partial f}{\partial \mathbf{q}} = \frac{\partial H}{\partial \mathbf{p}} \cdot \frac{\partial f}{\partial \mathbf{q}} - \frac{\partial H}{\partial \mathbf{q}} \cdot \frac{\partial f}{\partial \mathbf{p}} = 0 \quad (3.21)$$

We call the expression appearing on the right hand side of the second equality the Poisson bracket of  $f$  and  $H$  CITE AL GOLDSTEIN, and we abbreviate it as  $\{f, H\}$ . Using this definition, we have a condition for a function  $f$  to be a constant of motion when the Hamiltonian does not depend on time CITE ZASLAVSKI HAMILTONIAN CHAOS AND FRACTIONAL DYNAMICS:

$$\{f, H\} = 0. \quad (3.22)$$

(The Hamiltonian is a constant of the motion since  $\{H, H\} = 0$ .)

For a system with  $N$  degrees of freedom to be integrable, in the Liouville sense, it is necessary to exist  $N$  constants independent of movement (or motion)  $f_i(\bar{p}, \bar{q})$  (CITE DE PAGINA: If a constant cannot be described as a function of others, then it is called "independent" CITE OTT DYNAMICAL), with  $i = 1, 2, \dots, N$  in such a way that

$$\{f_i, H\} = 0 \quad (3.23)$$

and

$$\{f_i, f_j\} \delta_{ij} \quad (3.24)$$

where  $\delta_{ij}$  is the kronecker delta, for all  $i$  and  $j$  CITE HAMILTONIAN CHAOS AND FRACTIONAL DYNAMICS ZASLAVSKI. Said in another way, the vectors  $\mathbf{v}_i$ , defined by

$$\mathbf{v}_i = \nabla f_i, \quad (3.25)$$

where  $\nabla = (\partial/\partial q_1, \dots, \partial/\partial q_N, \partial/\partial p_1, \dots, \partial/\partial p_N)$  is the nabla operator of phase space, must be linearly independent at all the points in phase space CITE LIBRO DE MECANICA ANALITICA QUE DIGA ESO. If the conditions (3.23)-(3.25) apply to any  $i$  and  $j$ , then we

say that the  $N$  constants of motion are in involution.

When an  $N$  dimensional Hamiltonian system is integrable possessing  $N$  independent constants of motion, the topology of the surface on which its trajectories evolve in the phase space are restricted to an  $N$  dimensional torus CITE HAMILTONIAN CHAOS AND FRACTIONAL DYNAMICS ZASLAVSKI. For the case  $N = 2$ , an orbit over a torus is shown in Figure (3.2)

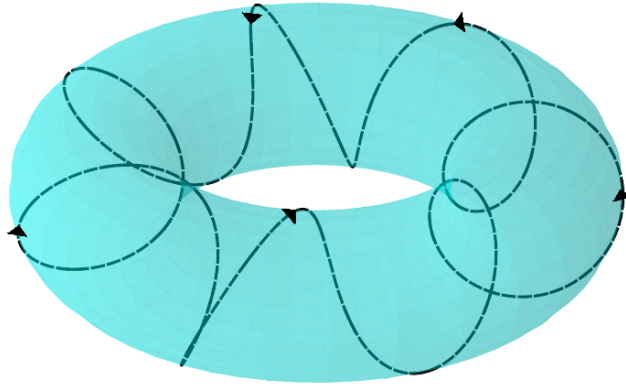


Figura 3.2: Trajectory on a torus for a bidimensional system with two constants of motion

A simpler description of the movement of integrable Hamiltonian systems over the  $N$  dimensional torus, can be made using the description in terms of the action-angle variables and the Hamilton-Jacobi equations, whose formalism can be found in Ref. CITAR AL GOLDSTEIN. For this, a canonical change of variables  $(\mathbf{p}, \mathbf{q}) \rightarrow (\tilde{\mathbf{p}}, \tilde{\mathbf{q}})$  is introduced such that the Hamiltonian  $\tilde{H}$  depends only on  $\tilde{\mathbf{p}}$  and not on  $\tilde{\mathbf{q}}$ . This way, the Hamilton's equations with the new Hamiltonian become

$$\frac{d\tilde{\mathbf{p}}}{dt} = -\frac{\partial \tilde{H}}{\partial \tilde{\mathbf{q}}} = 0 \quad \text{and} \quad \frac{d\tilde{\mathbf{q}}}{dt} = \frac{\partial \tilde{H}}{\partial \tilde{\mathbf{p}}} \quad (3.26)$$

and  $H(\mathbf{p}, \mathbf{q})$  becomes  $\tilde{H}(\tilde{\mathbf{p}})$ .

Using the action-angle variables, we will write the components of the moment  $\tilde{\mathbf{p}}$  and of the generalized coordinates  $\tilde{\mathbf{q}}$  as

$$(\tilde{\mathbf{p}}, \tilde{\mathbf{q}}) = (\mathbf{I}, \boldsymbol{\theta}), \quad (3.27)$$

where the components of the action  $\mathbf{I}_i$  are defined by CITAR AL GOLDSTEIN

$$\mathbf{I}_i = \frac{1}{2\pi} \oint p_i dq_i \quad \text{where} \quad i = 1, 2, \dots, N. \quad (3.28)$$

This way, we are writing the components of  $\tilde{\mathbf{p}}$  as being  $N$  constants of motion and at the same time satisfying Eq. (3.26), since the time variation of a motion constant is zero.

In order to achieve the change of variables  $(\mathbf{p}, \mathbf{q}) \rightarrow (\mathbf{I}, \boldsymbol{\theta})$ , we use the generating function  $S(\mathbf{I}, \mathbf{q})$  and the relations CITAR AL GOLDSTEIN

$$\boldsymbol{\theta} = \frac{\partial S(\mathbf{I}, \mathbf{q})}{\partial \mathbf{I}} \quad \text{and} \quad \mathbf{p} = \frac{\partial S(\mathbf{I}, \mathbf{q})}{\partial \mathbf{q}} \quad (3.29)$$

because this function relates the “old” coordinates of the position  $\mathbf{q}$  and the “new” moment  $\mathbf{I}$  CITAR AL GOLDSTEIN. With this, we can construct the Hamiltonian function in terms of the action-angle variables,  $\tilde{H}(\mathbf{I})$  which is independent of  $\boldsymbol{\theta}$ .

As said in the last paragraph, the new Hamiltonian is independent of  $\boldsymbol{\theta}$  and the Hamilton equations Eq. (3.26), can be written as

$$\frac{d\mathbf{I}}{dt} = 0 \quad \text{and} \quad \frac{d\boldsymbol{\theta}}{dt} = \frac{\partial \tilde{H}(\mathbf{I})}{\partial \mathbf{I}} \equiv \boldsymbol{\omega}(\mathbf{I}), \quad (3.30)$$

their solutions are

$$\mathbf{I}(t) = \mathbf{I}(0) \quad (3.31)$$

and

$$\boldsymbol{\theta}(t) = \boldsymbol{\theta}(0) + \boldsymbol{\omega}(\mathbf{I})t \quad (3.32)$$

where each angle variable is periodic with a period of  $2\pi$ .

The second equation in Eq.(3.30) can be interpreted as an angular velocity vector specifying trajectories over the  $N$  dimensional torus CITAR AL GOLDSTEIN, where  $\mathbf{I}$  represents the radius of the trajectory and  $\boldsymbol{\theta}$  the angle of rotation. this fact is illustrated in Fig. FIGURA QUE NO HE HECHO DE LA SECCION TRANSVERSAL DEL TORO for the case where  $N = 2$ . With the interpretation of  $\boldsymbol{\omega}(\mathbf{I})$  as an angular velocity vector that specifies different paths over an  $N$  dimensional torus, different types of movement over the torus can occur, which may be periodic or quasi-periodic, depending on the ratio between these frequencies. If there is an  $N$  dimensional vector of integers  $\mathbf{m} = (m_1, m_2, \dots, m_n)$ , such that

$$\mathbf{m} \cdot \boldsymbol{\omega} = 0, \quad (3.33)$$

except when  $\mathbf{m}$  is a vector with all null components, the movement over the torus is a periodic movement and the ratio  $\omega_1/\omega_i$  is a rational number. In these cases, the orbits followed by the system close on themselves after  $m_1$  cycles in  $\theta_1$ ,  $m_2$  cycles in  $\theta_2$  and so on [? ]. When condition (3.33) is not satisfied and  $\omega_1/\omega_i$  is an irrational number, the motion of the system is called quasi-periodic and an orbit never returns to its starting point, completely filling the surface of the torus [? ].

When an integrable system begins to suffer the action of a disturbance, the tori whose ratio between frequencies is a rational or irrational number, behave in different ways. The consequences of this disturbance on such tori are explained by the KAM theorem, which we will describe later.

### 3.2.2. KAM Theorem

In the last subsections we introduced the necessary conditions for a system to be integrable. We also found that when the Hamiltonian is written in terms of the motion constants, especially in relation to the angle-action variables, the system's movement is limited to a rational or irrational  $N$  dimensional torus, depending on the frequencies of the motion. But where does the integrability of a Hamiltonian system go? Or yet, what happens to rational and irrational tori when an integrable Hamiltonian system is subject to a disturbance? The answers to these questions came with the rigorous mathematical work of Kolmogorov, Arnold and Moser (KAM) and with the numerical studies developed on chaos and integrability after the advent of computer. The results obtained by Kolmogorov, Arnold and Moser became known as the KAM Theorem. The deduction of the theorem will not be detailed here, as it is outside the scope of this work, only its results will be presented.

To describe the KAM theorem, we consider a disturbed Hamiltonian system, written in terms of the action-angle variables as

$$H(\mathbf{I}, \boldsymbol{\theta}) = H_0(\mathbf{I}) + \epsilon H_1(\mathbf{I}, \boldsymbol{\theta}), \quad (3.34)$$

where  $H_0(\mathbf{I})$  is the integrable Hamiltonian,  $H_1(\mathbf{I}, \boldsymbol{\theta})$  the perturbation and  $(\mathbf{I}, \boldsymbol{\theta})$  the action-angle variables of perturbed system.

The main idea of the KAM Theorem is to consider the effect of the disturbance on invariant Tori. A TORUS IS CALLED INVARIANT IF ONCE THE MOTION OF THE SYSTEM STARTS ON IT, THE MOTION STAYS ON IT. CITE OTT DYNAMICAL SYSTEMS. instead of the trajectories in the phase space CITE CHAOS AND FRACTIONAL DYNAMICS ZASDKJASD. In this way, we will divide the discussion into two cases, the

Rational Torus and the Irrational Torus. We will see that many tori survive small disturbances, while others destroy themselves, giving rise to chaotic orbits, new tori and also elliptical and hyperbolic points.

### 3.2.3. Rational Tori

We call Rational Tori those whose ratio between the frequencies given by Eq.(3.30) is a rational number. As a result of the action of the disturbance, these Tori are destroyed and it does not matter how small the values of  $\epsilon$  are [? ]. Due to the destruction of the Rational Torus, there is the appearance of an equal number of fixed elliptic and hyperbolic points. This result is known as the Poincare Birkhoff theorem CITE REGULAR AND CHAOTIC DYNAMICS LICHTENBERG LIEBERMAN . The number of fixed points that appear depends on the ratio between the frequencies of the rational torus. If we call  $R = \tilde{p}/\tilde{q}$  the torus rotation number, where  $\tilde{q}$  represents the largest number of cycles performed on the torus before the path returns over itself, then, due to the disturbance, there will appear an equal or multiple number of  $\tilde{q}$  of elliptical points and hyperbolic points [? ]. Fig. (FIGURA QUE NO HE HECHO DEL TORO RACIONAL PERTURBADO POCAMENTE) illustrates a case where  $\tilde{q} = 3$  and  $\tilde{p} = 4$  in a Poincare section for a system with  $N = 2$ .

These elliptical and hyperbolic points that result from the breakdown of the rational torus due to the perturbation, they remain fixed points of the disturbed system and with the same period  $\tilde{q}$  of the rational torus CITE REGULAR AND CHAOTIC DYNAMICS LICHTENBERG LIEBERMAN . The difference between the two points is in the way initial conditions close to them behave. Next to fixed elliptical points, new curves appear similar to those that existed before the perturbation, which we call KAM curves, some of which are rational and others irrational. Such fact is presented inside the box on Fig. (FIGURA ANTERIOR LA PARTE B TIENE UNA CAJA CERRADA DE UN PUNTO ELIPTICO). When these rational KAM curves that appeared due to the action of the disturbance are destroyed, other elliptical and hyperbolic points will appear, surrounded again by rational and irrational KAM curves and so on [? ].

Orbits generated near hyperbolic points, can have different behaviors, because hyperbolic points, also known as saddle points, have stable directions or varieties, those that move to the fixed point, or unstable, those who move away from it [? ]. If we follow the varieties, moving away from a fixed point, they will usually present homoclinic or heteroclinic intersections, which occur when unstable varieties from the same point cross over themselves or from two different points intersect at different points, respectively [? ]. Fig. (REF FIGURA QUE NO HE HECHO DE LOS ENREDAMIENTOS HOMOCLINICOS) represents these crossings for

a single point and for two distinct hyperbolic points.

Thus, the destruction of the rational torus not only generates stable elliptical points, but also generates hyperbolic points, which are responsible for the chaotic movement, which is always trapped by the KAM curves that haven't been "broken" [? ], at least for an  $N = 2$  case. As these curves begin to "break", more and more chaotic regions are appearing, completely filling with points the allowed region of the Poincare section. We will now see what is the sequence in which the irrational torus gives rise to the elliptical and hyperbolic points. FIGURA

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### 3.2.4. Irrational Tori

When an integrable system is disturbed, the KAM Theorem guarantess the existence of a torus in the phase space, if te conditions below are met:

1. The torus' linear frequencies of the integrable system are independent CITE REGULAR AND CHAOTIC DYNAMICS LICHTENBERG LIEBERAN, that is, we hae a torus whose ratio between the frequencies is an irrational number.
2. The perturbation is a smooth function CITE REGULAR AND CHAOTIC DYNAMICS LICHTENBERG LIEBERAN (a sufficient number of derivaties of  $H_1$ ).
3. Initial conditions are sufficiently far from the rational tori CITE REGULAR AND CHAOTIC DYNAMICS LICHTENBERG LIEBERAN.

With the above conditions satisfied, the KAM Theorem guarantess the existence of deformed torus, with the same topology as the unperturbed torus, in the vicinity of te irrational torus of the system in the non-perturbed. These tori that appear deformed after the perturbation are called the KAM Tori.

The that the irrational torus must be sufficiently far from the rational torus, for the existence of the KAM Tori, implies that the more irrational the ratio between the frequencies of the non-perturbed tori, the easier it is for the KAM Tori to appear CITE REGULAR AND CHAOTIC DYNAMICS LICHTENBERG LIEBERAN.

The idea of more irrational numbers can come with the help of number theory. An irrational number  $R$  can be represented as an infinite continuous function [? ]:

$$R = a_1 + \frac{1}{a_2 + \frac{1}{a_3 + \frac{1}{a_4 + \dots}}} \quad (3.35)$$

where the  $a_i$ 's are integer numbers. However, if the integers  $a_i$ 's for  $i \geq k$  are equal to one, this irrational number is called “noble” CITE ORDER AND CHAOS IN DYNAMICAL ASTRONOMY CONTOPOULOS. The “most irrational” number that exists is consequently the most “noble” of them all CITE ORDER AND CHAOS IN DYNAMICAL ASTRONOMY CONTOPOULOS, and it is the golden ratio

$$R = \frac{(\sqrt{5} - 1)}{2} \quad (3.36)$$

When the most “noble” number of all is related to the irrationality of a KAM Tori, it will be the last one to be destroyed as the intensity of the perturbation is increased. However, if it is not present, the last KAM Tori to be destroyed will be the one with the most “noble” number CITE ORDER AND CHAOS IN DYNAMICAL ASTRONOMY CONTOPOULOS.

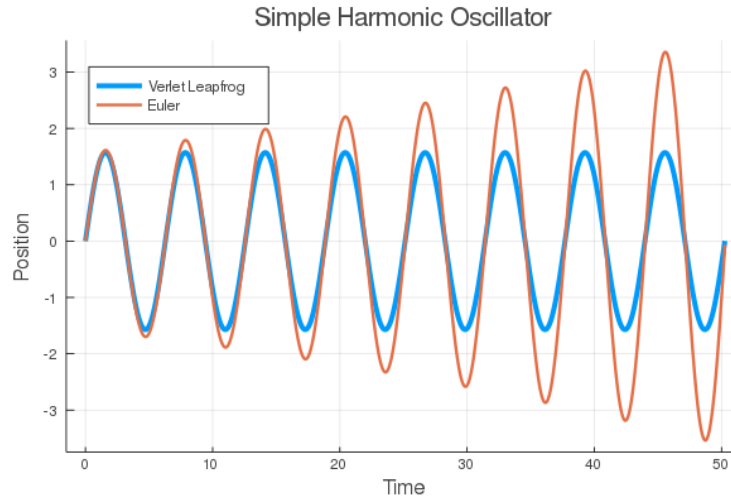
In general, the effect of the perturbation on an integrable system can be summarized as follows: When the disturbance begins to act on the integrable system, many tori of the integrable system are slightly deformed and survive (Irrational Tori), while others are destroyed (Rational Tori). Regions close to the tori that were not destroyed by the perturbation are occupied by new irrational orbits, elliptical points, hyperbolic orbits and chaotic orbits. As the disturbance increases, the irrational tori destroy themselves, the last one to be “destroyed”, is the one that has the value of the ratio between the frequencies as a “more noble” number.

When the perturbation on the integrable system breaks all tori, including the “noblest”, the system starts to present characteristics such as ergodicity, drops of correlations, etc...

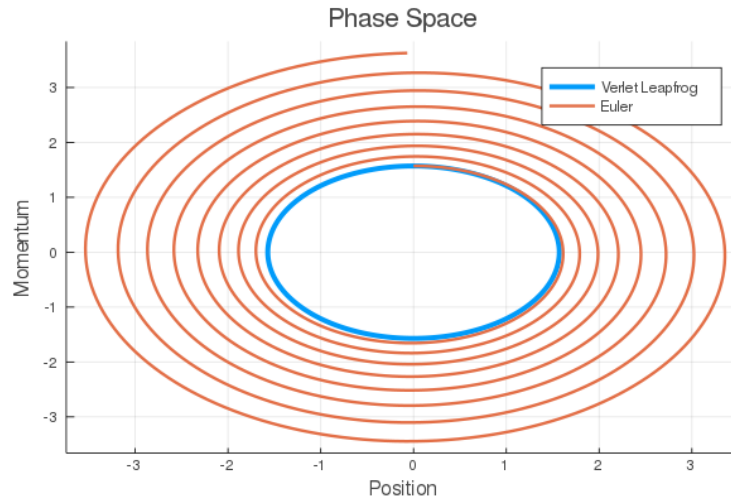


### 3.3. Symplectic Integrator NUMERICAL HAMILTONIAN PROBLEMS

As we said previously, symplecticness is a very important property of the Hamiltonian. Numerical integrators are generally speaking numerical mappings of the differential equations, generally these mappings are nonsymplectic. Applying nonsymplectic algorithms to hamiltonian problems tend to show solutions where the area in phase space is not conserved as is showed below



((a)) Position dynamics



((b)) Phase space dynamics

Figura 3.3: Euler non symplectic integrator compared to symplectic Verlet Leapfrog method

This failure of mimicking well known Hamiltonian dynamics suggested the consideration

of schemes that generate a symplectic mapping  $Psi$  when applied to Hamiltonian problems. Such methods are called symplectic or canonical. Early references on symplectic integration are CITAR A RUTH CHANNEL MENYUK FENG, even though the idea of symplectic integration apparently goes back to DeVogelaere in 1956 CITAR CHANNEL SCOVEL 1990.

### 3.3.1. Importance of symplecticness in an integrator

A symplectic integrator is then an integrator whose solution resides on a symplectic manifold. Because of discretization error, when it is solving a Hamiltonian system it doesn't get exactly the correct trajectory on the manifold. Instead, that trajectory itself is perturbed  $\mathcal{O}(\Delta h^n)$  for the order  $n$  from the true trajectory. Then there's a linear drift due to numerical error of this trajectory over time. Normal integrators tend to have a quadratic (or more) drift, and do not have any good global guarantees about this phase space path, it only guarantees the path in a local sense.

What this tends to mean is that symplectic integrators tend to capture the long-time patterns better than normal integrators because of this lack of drift and this almost guarantee the periodicity of certain problems.

### 3.3.2. Conservation of constants of motion

As we have seen previously, when one uses a symplectic integrator of order  $n$  what you do is to solve in an exact way the evolution of the system, but not using the hamiltonian  $H$  but one softly perturbed as  $\tilde{H} = H + \epsilon H_1$ , where  $\epsilon = t^n$  and  $H_1 = H_1^0 + hH_1^1 + h^2H_1^2 + \dots$ . If what we really want to obtain is a qualitative information of the behavior of the system, we can expect that if  $\epsilon H_1$  is sufficiently small, the system will evolve in a very similar way for  $\tilde{H}$  as for  $H$ .

Consider now a system that has  $m$  independent constants of motion  $J_i$  where  $i = 1, \dots, m$ , this means that for every  $J_i$  it satisfies the condition of a null poisson bracket with the hamiltonian as  $\{H, J_i\} = 0$ . As the integrator is solving in an exact way the evolution due to the hamiltonian  $\tilde{H}$ , it will follow that the constants of motion, in general, will not be constant as they will not have a null poisson bracket, in principle, with this new hamiltonian. Nonetheless, the following is obtained

$$\{\tilde{H}, J_i\} = \{H + \mathcal{O}(h^n), J_i\} = \mathcal{O}(h^n). \quad (3.37)$$

Despite some exceptions, the constants of motion  $J_i$  will not be constant along the evolution of the system, but they will disagree to being it in the same order as the energy does. Therefore,

for an efficient integrator with high order precision the constants of motion will certainly be constant along the dynamical trajectory.

### 3.3.3. Chaos and integrators TOCA METERLE VARIAS REFERENCIAS

Numerical chaos has been a very interactive branch of study for many years since the surge of computers. As we have shown, numerical stability of differential equations is very sensitive to systems involving chaos, even the slightest difference on the floating point error gives rise to diverging trajectories in phase space, this makes chaotic systems very interesting problems numerically speaking. As we know, floating numbers that computer algorithms work with have a finite value for decimals, when computing a solution of a differential equation using a given algorithm computers truncate this decimals leaving some round-off error. These truncations are not overseen by chaotic systems, chaotic systems has the nature to amplify the slightest perturbation of the system into an observable result, this means that numerical truncations on floating point numbers have long term consequences when interpreting what we consider the solution. It is necessary to take into account these considerations when solving a chaotic system.

Numerical integrators and chaos consequently gather on an exotic dance of conditions to consider, on one hand it is important for integrators to have a high order of accuracy by using intermediate steps before computing a definitive step on the trajectory of the solution and it is also important to have a small enough integration step to manage sensibility for the trajectory; on the other hand, error propagation of the floating point decimal truncation everytime the integrator performs an operation discourages all the effort put into calculating derivatives using intermediate steps and raises the question on what is the important aspect to consider. The answer is often unknown, solving these numerical problems with optimal efficiency is truly a very complicated task for the majority of chaotic problems.

## 3.4. Randomness in classical and quantum mechanics

Randomness and chaos share similarities physically speaking, they amplify any type of noise from the microscopical degrees of freedom and show them visible in the outcome of the dynamics of the systems. The idea to achieve true randomness on experiments or random number generators is a dream for many experimentalists, but the true situation is that most of the times, classically you can't have the perfect un-biased scenario

of randomness. One great example is illustrated by Diaconis et al. CITAR PAPER DIACONIS MONEDA where very precise measurements and theoretical descriptions are applied to the commonly known random event of the coin toss. The outcome of this research is that for natural flips the result of the coin is biased to come up as started

51Li, Pu; Sun, Yuanyuan; Liu, Xianglian; Yi, Xiaogang; Zhang, Jianguo; Guo, Xiaomin; Guo, Yanqiang; Wang, 07–15).” *Fully photonic-based physical random bit generator*. *Optics Letters*, 41(14) : 3347–3350. Bibcode : 2016OptL...41,3347L. doi : 10.1364/OL.41.003347. ISSN 1539–4794. PMID 27420532. ), *it has a high potential speed random numbers due to its high bandwidth and large amplitude. A prototype of a high speed, real-time physical random bit generator based on a chaotic laser was built in 2013 CITARA* (Wang, Anbang; Li, Pu; Zhang, 08–26).” *4.5 Gbps high-speed real-time physical random bit generator*. *Optics Express*, 21(17) : 20452–20462.).

Determinism defined as the property of events to be determined completely by previously existing causes is an important concept concerning classical mechanics, given the equations of motion of a system, we know in an exact way the state of the system in a future time with arbitrary precision. Chaotic systems are very sensitive to small changes on the initial conditions and they are often misunderstood as random, but as we have previously described, chaotic systems do not exhibit random behavior in the sense that it can be at any place located in phase space but we have shown that it certainly remains conditioned by a certain degree to the motion on the KAM tori giving place to quasiperiodicity.

On the other hand, quantum mechanics seems to have fundamental randomness in its roots, measurements are regarded as probability measurements of the system to be in a determined state. The Born’s interpretation of the quantum mechanics of the wave function implies that we can count only on a probabilistic description of reality, therefore quantum mechanics is inherently probabilistic CITAR LA INTERPRETACION DE BORN DE QM. Randomness in quantum mechanics is also regarded to be due to the interaction of a measurement apparatus and an environment with the initial pure states. This is consistent and parallel to the modern way of interpretations of the collapse of the wave functions and the quantum measurements CITAR A WHEELER AND ZUREK 1983 ZUREK 2003 Y ZUREK 2009.

It is important for us to talk about the experiment to measure a spin component along a direction. If we take the  $z$  component as an example similar to the Stern-Gerlach experiment CITAR EL EXPERIMENTO DE STERN GERLACH, in this experiment the particles before the measurement are regarded to be in a neutral state along the  $z$  component, after the particles go through the inhomogeneous magnetic field the spin aligns along a direction of the  $z$  component and gets deflected along this direction. The result of the experiment is seen in a screen where two clouds of particles are seen, one in the upper location and one in the lower

one. The counts of particles on each cloud is the same in both cases, this translates as the probability of the particles to be aligned along certain direction is the same. Particles then have a completely random probability to be aligned along certain direction, this idea can be compared with the one of the coin toss, only two possible outcomes of the measurement. There is a big difference between both pictures besides one being classical and the other one quantum, it is that the coin toss is not truly random as it depends strongly on the initial conditions on how the coin toss is made meanwhile the spin measurement seems to be totally random as long as the particle is initially in a non-commuting state with the  $z$  component of the spin. This idea is the one we are going to exploit on the next chapters and explore a little bit the grounds of the environment and its role of introducing bias to the outcome of the measurements.



# DOUBLE WELL AND FINITE HEAT BATH

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In this chapter we will use a model to test the interaction between a particle on a double well potential coupled bilinearly on position with a bath consisting of harmonic oscillators. This model is initially chaotic following the rules we have stated on the previous chapters regarding chaotic motion. The difference here with the previous chapters is that we will increase the number of degrees of freedom in the whole system by increasing the number of harmonic oscillators in the heat bath.

The main results of this chapter are related to the theory of dissipative dynamics in open systems but with a finite number of oscillators in the heat bath. We will play with different parameters of the heat bath such as energy and frequencies following this matter.

## 4.1. Double well as a two level system

### 4.1.1. Quantum modeling for continuous variables

### 4.1.2. Heat bath proper modeling

## 4.2. Dynamics of the system

### 4.2.1. Hamilton equations of motion

This system is governed by the following hamiltonian:

$$H(p, x; \mathbf{P}, \mathbf{X}) = H_S + H_B + H_{SB} \quad (4.1)$$

Where the hamiltonian for the central system ( $S$ ) can be viewed as a particle of mass  $m$  moving in a double well potential of quartic nature. The corresponding hamiltonian reads as

$$H_S = \frac{p^2}{2m} - a\frac{x^2}{2} + b\frac{x^4}{4}, \quad (4.2)$$

where  $p$  is the momentum of the particle,  $q$  is the position of the particle, and  $a, b$  are parameters that change the shape of the potential. The hamiltonian for the bath ( $B$ ) is described as a set of harmonic oscillators

$$H_B(\mathbf{P}, \mathbf{X}) = \sum_{n=1}^N \left( \frac{P_n^2}{2M_n} + M_n \omega_n^2 \frac{X_n^2}{2} \right), \quad (4.3)$$

each oscillator  $n$  possesses position  $X_n$ , momentum  $P_n$ , frequency  $\omega_n$  and mass  $M_n$ . The last term of the hamiltonian consists of the interaction term where the system and bath positions are coupled bilinearly according to

$$H_{SB}(p, x; \mathbf{P}, \mathbf{X}) = -x \sum_{n=1}^N g_n X_n + x^2 \sum_{n=1}^N \frac{g_n^2}{2M_n \omega_n^2} \quad (4.4)$$

The last term here acts as a counter term whose job is to renormalize the potential when the interaction between the oscillators is present. This hamiltonian is often called the Caldeira-Leggett hamiltonian CITAR POR QUE LLAMAN CALDEIRA LEGGETT.

The hamilton equations for this hamiltonian can be separated in the two parts, the particle and the heat bath. The hamilton equations of the particle read as

$$\dot{p} = \frac{-\partial H}{\partial x} = ax - bx^3 + \sum_{n=1}^N g_n X_n - x \sum_{n=1}^N \frac{g_n^2}{M_n \omega_n^2}, \quad (4.5)$$

$$\dot{x} = \frac{\partial H}{\partial p} = \frac{p}{m}. \quad (4.6)$$

For the heat bath we find that the equations of motion for each of the  $n$  oscillators are given by

$$\dot{P}_n = \frac{-\partial H}{\partial X_n} = -x g_n - M_n \omega_n^2 X_n \quad (4.7)$$

$$\dot{X}_n = \frac{\partial H}{\partial P_n} = \frac{P_n}{M_n} \quad (4.8)$$

From these equations we can calculate the frequency of small oscillations for the double



well potential, we proceed by taking the the potential given as

$$V(x) = -\frac{1}{2}ax^2 + \frac{1}{4}bx^4, \quad (4.9)$$

the equilibrium points are located where the potential  $V$  is minimum or maximum, this is when the following condition is satisfied

$$\frac{d}{dx}V = 0 \rightarrow x(bx^2 - a) = 0. \quad (4.10)$$

The solutions for this equation are  $x = 0, \pm\sqrt{\frac{a}{b}}$ , where  $x = 0$  is an unstable equilibrium point and  $x = \pm\sqrt{\frac{a}{b}}$  are stable equilibrium points

We proceed to perform a Taylor expansion around a stable equilibrium point say  $x_0 = \sqrt{\frac{a}{b}}$  as

$$V(x_0 + \epsilon) = V(x_0) + U'(x_0)\epsilon + \frac{1}{2}V''(x_0)\epsilon^2 + \dots \quad (4.11)$$

The first term on the right side is a constant term, this means it can be ignored. The second term is equal to zero due to the fact that  $V'(x_0) = 0$  is the condition for the stable minimum. The third term will be according to the result of  $V''(x_0) = \frac{1}{2}(-a + 3bx^2)|_{x=x_0}$ , this results in the following expansion

$$V(x_0 + \epsilon) \approx \frac{1}{2}(2a)\epsilon^2. \quad (4.12)$$

This potential is the same expression of a harmonic oscillator potential with a spring constant of  $k = 2a$  (compared with the harmonic oscillator potential  $V_{HO} = \frac{1}{2}kx^2$ ). This means that the frequency of small oscillations around the stable minimum is given by

$$\omega = \sqrt{\frac{k}{m}} = \sqrt{\frac{2a}{m}} \quad (4.13)$$

For the case of the particle coupled to the heat bath we can do the same analysis and see the role of the counter term in the hamiltonian resulting in the same results as above. The equilibrium points of the whole hamiltonian must satisfy the following condition

$$\frac{d}{d\mathbf{x}}H = 0 \rightarrow \frac{d}{dx}H = 0 \quad , \quad \frac{d}{dX_n}H = 0. \quad (4.14)$$

Evaluating the derivatives we arrive to the following equations

$$x(bx^2 - a) - \sum_{n=1}^N g_n X_n + \sum_{n=1}^N \frac{xg_n^2}{M_n\omega_n} = 0 \quad , \quad xg_n = M_n\omega_n^2 X_n \quad (4.15)$$

where the right hand side equation will provide the constraint to retrieve the original conditions of equilibrium for the potential on the right hand side

$$x(bx^2 - a) - \sum_{n=1}^N g_n X_n + \sum_{n=1}^N \frac{x g_n^2}{M_n \omega_n} = x(bx^2 - a) - \sum_{n=1}^N g_n X_n + \sum_{n=1}^N g_n X_n = x(bx^2 - a) = 0. \quad (4.16)$$

We can also calculate the height of the potential barrier (the difference between the height of the unstable equilibrium with the stable equilibrium), we can do this by insterting one of the minima on equation (4.9):

$$V(\sqrt{\frac{a}{b}}) = -a \frac{a}{2b} + b \frac{a^2}{4b^2} = \frac{-a^2}{2b} + \frac{a^2}{4b} = -\frac{a^2}{4b}, \quad (4.17)$$

For this particular situation the unstable equilibrium is located at the 0 height, meaning that in general the height of the potential barrier will be the difference between the unstable and the equilibrium point given as

$$PB(a, b) = \frac{a^2}{4b} \quad (4.18)$$

### 4.2.2. Infinite heat bath and dissipation

### 4.2.3. Poincaré surface plots

We start the numerical experiments of this model with only one oscillator coupled to the particle of the central system. This very simple model already exhibits the traits and characteristics of a chaotic system, this is due to the barrier of the unstable equilibrium position. We can illustrate this by picturing the particle moving on the double well potential without any coupling with the heat bath, if the particle has enough energy, it will move freely between the two wells, otherwise it will orbit around one well. This can be seen in two different ways, the first one is by looking at the potential part of the hamiltonian of each part of the whole system i.e. the quartic potential and the harmonic oscillator potential, plotting each potential along an axis we can see the contours of energy for the dynamics of the system.

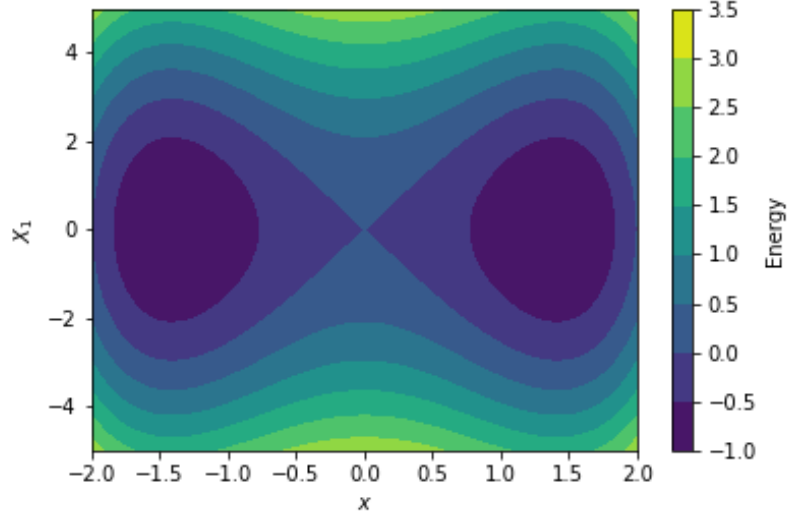


Figura 4.1: Energy contour of the double well potential on the  $x$  axis and the harmonic oscillator potential on the  $y$  axis for  $m = 1$ ,  $a = 2$ ,  $b = 1$ ,  $\omega_1 = 1,5$ ,  $M_1 = 0,1$  and  $g_1 = 0$

In Figure (4.1) we see that as the dynamics is uncoupled, the particle moves freely on the double well potential and the harmonic oscillator doesn't really changes its motion.

Following this representation we can observe the perturbation induced by the harmonic oscillator when we "turn on" the coupling between the two systems, for a coupling of  $g_1 = 0,1$  it is already evident that shape of the whole potential suffers a shearing effect:

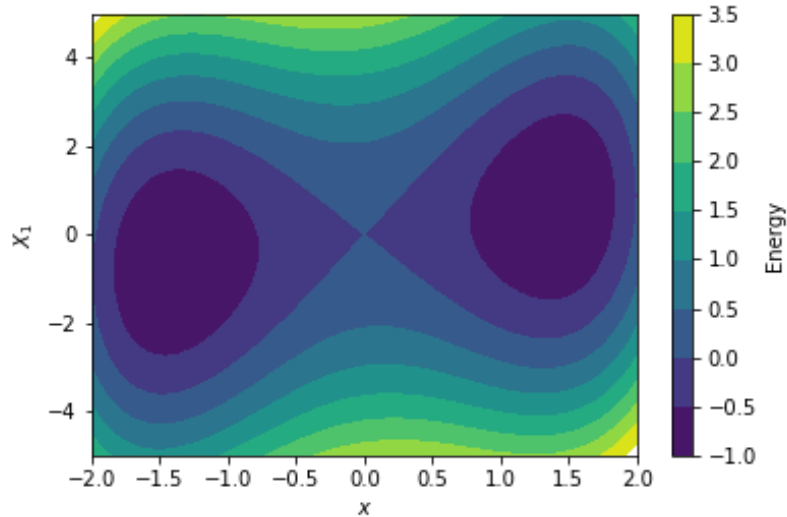


Figura 4.2: Energy contour of the double well potential on the  $x$  axis and the harmonic oscillator potential on the  $y$  axis for  $m = 1$ ,  $a = 2$ ,  $b = 1$ ,  $\omega_1 = 1,5$ ,  $M_1 = 0,1$  and  $g_1 = 0,1$

This means that independently of the initial conditions of the particle, the motion will be certainly affected by the presence of the potential due to the harmonic oscillator.

Now that we have seen a visual representation of the system without solving the equations of motion of the system, it is necessary to take a look at the specific dynamics of the system numerically by using a symplectic integrator. The integrator of our choice is the Calvo Sanz-Serna 4th order symplectic integrator CITAR

Stephen K. Gray, Donald W. Noid and Bobby G. Sumpter, Symplectic integrators for large scale molecular dynamics simulations: A comparison of several explicit methods The Journal of Chemical Physics 101, 4062 (1994); doi: <https://dx.doi.org/10.1063/1.467523>

M. P. Calvo J. M. Sanz-Serna, Symplectic numerical methods for Hamiltonian problems, Int. J. Mod. Phys. C 4(1993), 617-634

Rackauckas, C. Nie, Q., (2017). DifferentialEquations.jl – A Performant and Feature-Rich Ecosystem for Solving Differential Equations in Julia. Journal of Open Research Software. 5(1), p.15. DOI: <https://doi.org/10.5334/jors.151>

, we use a timestep defined by  $dt = 0,05 * T$  where  $T = \frac{2\pi}{\omega_t}$  is the period of a harmonic oscillator of frequency  $\omega_t = 12$ . Here we set up different initial conditions for the particle along its phase space, the position of the oscillator always to start at  $X_1 = 0$  and fixed the energy (twice the energy of the potential barrier between the wells here) as a constraint to be followed by the initial momentum of the oscillator. Each point of the poincaré section is registered as the event when the oscillator crosses its equilibrium position  $X_1 = 0$  with a positive momentum. We will take a number of initial conditions along the phase space of the particle and start to increase the coupling to see the behavior of the orbits in the phase space of the particle.

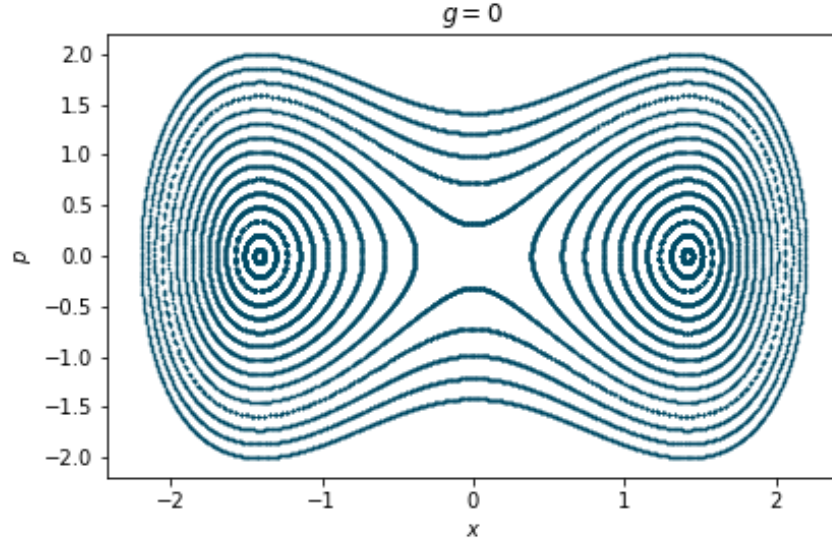


Figura 4.3: Poincaré surface plot for the particle phase space for  $m = 1$ ,  $a = 2$ ,  $b = 1$ ,  $\omega_1 = 1,5$ ,  $M_1 = 0,1$  and  $g_1 = 0$

In Figure (4.3) we start with  $g_1 = 0$  and see that the orbits on the phase space of the particle are closed, the particle is totally unaware of the harmonic oscillator's potential. Now we will slowly start to “turn on” the coupling between the systems.

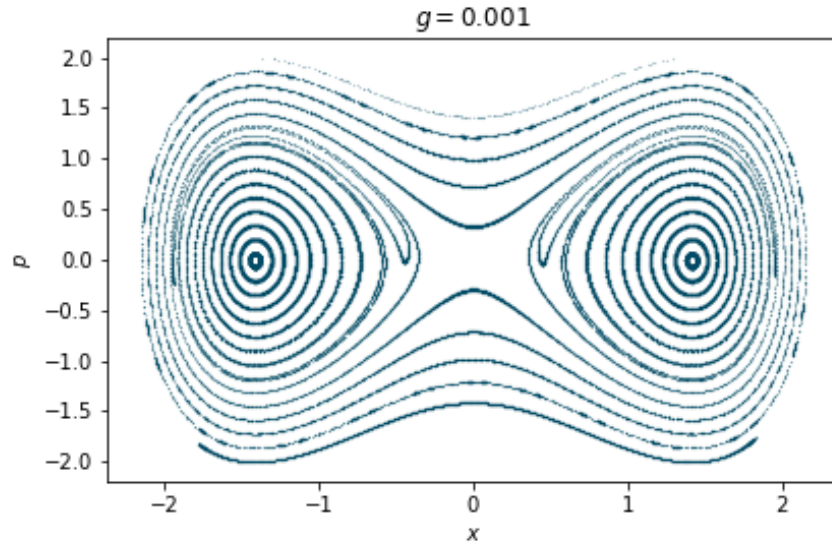


Figura 4.4: Poincaré surface plot for the particle phase space for  $m = 1$ ,  $a = 2$ ,  $b = 1$ ,  $\omega_1 = 1,5$ ,  $M_1 = 0,1$  and  $g_1 = 0,001$

As soon as there is coupling present in the dynamics of the system the orbits start to

destroy progressively as we can see in this Figure (4.4).

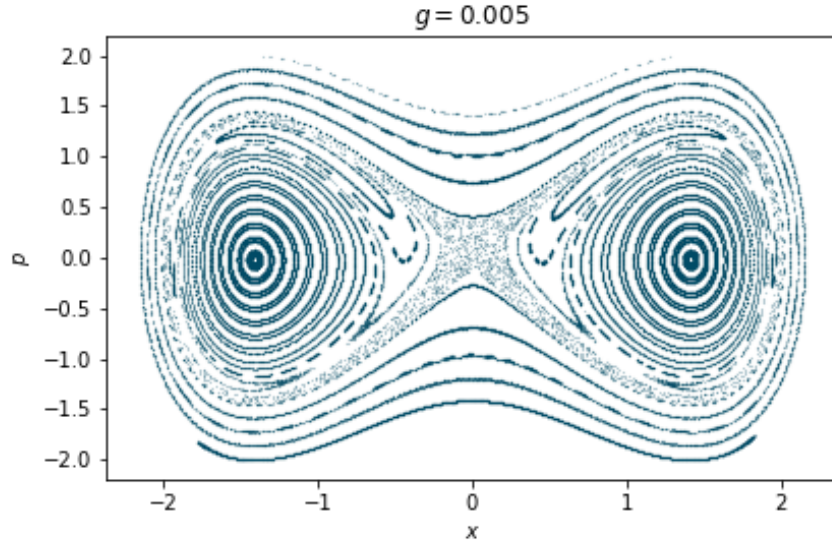


Figura 4.5: Poincaré surface plot for the particle phase space for  $m = 1$ ,  $a = 2$ ,  $b = 1$ ,  $\omega_1 = 1,5$ ,  $M_1 = 0,1$  and  $g_1 = 0,005$

The section of phase space where we start to see pure chaos at first is when the energy of the particle is very close to the energy of the barrier between the two wells as we can see in Figure (4.5), this particular behavior around this points is of particular interest for our case as we will later use the unstable equilibrium position as the initial condition for the particle.

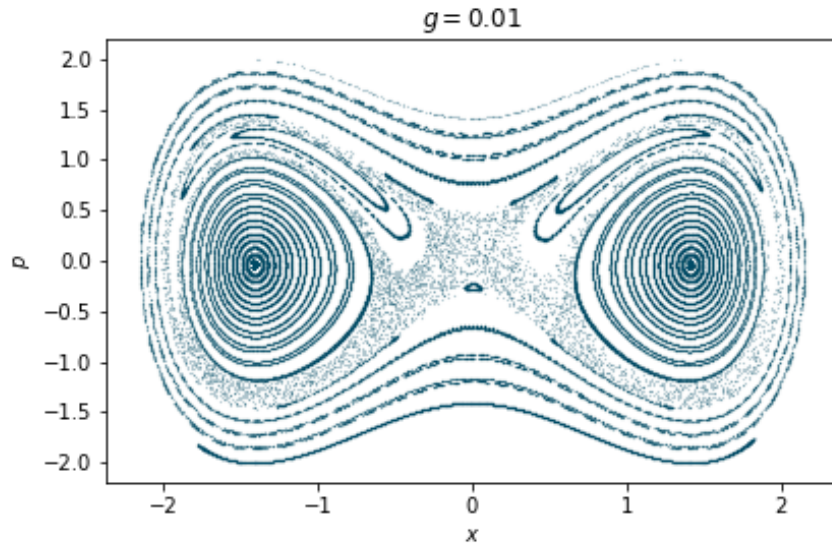


Figura 4.6: Poincaré surface plot for the particle phase space for  $m = 1$ ,  $a = 2$ ,  $b = 1$ ,  $\omega_1 = 1,5$ ,  $M_1 = 0,1$  and  $g_1 = 0,01$

As we continue to increase the coupling strength we progress on the destruction of the orbits and approach to a more chaotic behavior.

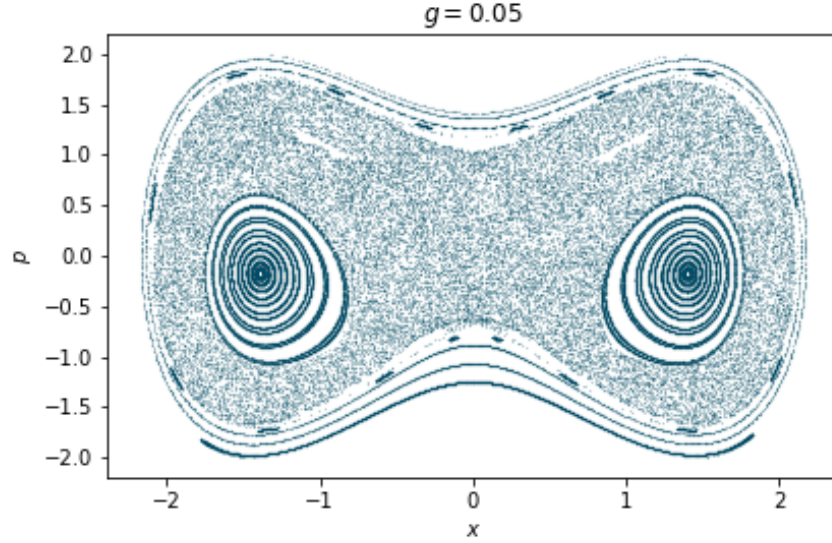


Figura 4.7: Poincaré surface plot for the particle phase space for  $m = 1$ ,  $a = 2$ ,  $b = 1$ ,  $\omega_1 = 1,5$ ,  $M_1 = 0,1$  and  $g_1 = 0,05$

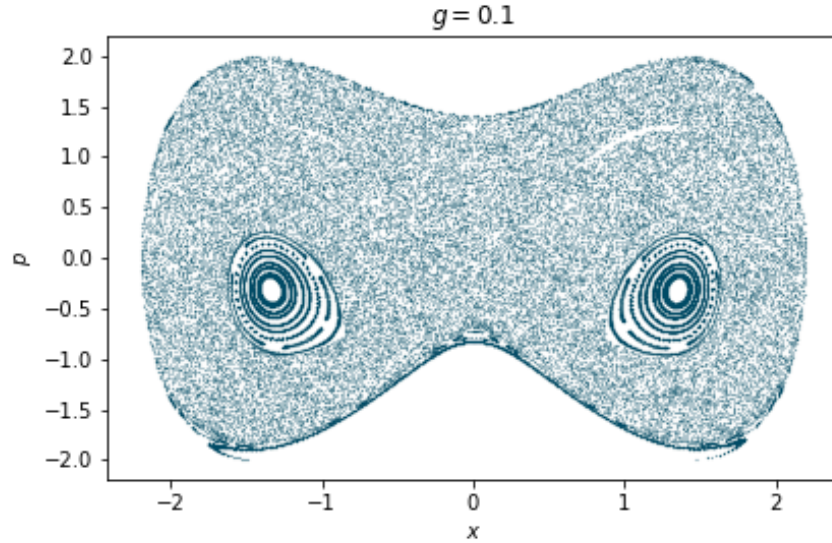


Figura 4.8: Poincaré surface plot for the particle phase space for  $m = 1$ ,  $a = 2$ ,  $b = 1$ ,  $\omega_1 = 1,5$ ,  $M_1 = 0,1$  and  $g_1 = 0,1$

Finally in Figure (4.8) we arrive to the coupling we used for Figure (4.2)  $g = 0,1$ . As we can see from the poincaré section, the overall behavior of the system is very chaotic except for



the stable islands very near to the condition of the particle to have small energy located near to the stable equilibrium points with a small momentum. Comparing these two pictures we can see that even if the shearing behavior observed in the contour plots can barely be noticed, the dynamics of the system is almost completely chaotic.

Just for illustration we calculated the poincare section for  $g = 0,2$  to show that the behavior of pure chaos continues to increase, this is shown in Figure (4.9).

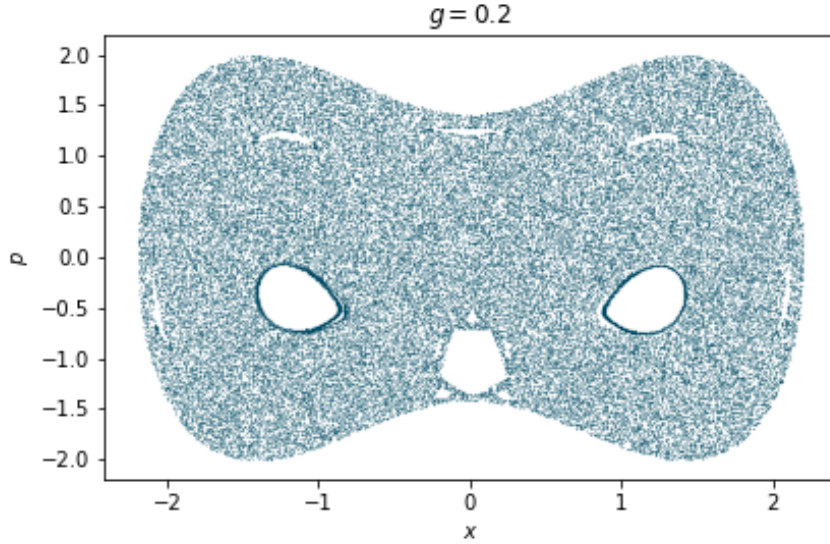


Figura 4.9: Poincaré surface plot for the particle phase space for  $m = 1$ ,  $a = 2$ ,  $b = 1$ ,  $\omega_1 = 1,5$ ,  $M_1 = 0,1$  and  $g_1 = 0,2$

### 4.3. Variation of the parameters

As it is evident, in this particular system we can vary a big amount of parameters to search for different dynamics and properties that exhibit the system, the model is rich in quantities that can be calculated and extracted from it. This idea also plays against our odds because as there are many parameters to play with it is difficult to control the whole system in an optimal and hierarchical way. There are two types of parameters that we will monitor very closely: the frequency spectra and the energy spectra for the heat bath.



### 4.3.1. Frequency spectra FALTA MUCHO POR ACABAR

The way the frequencies of the harmonic oscillators are distributed in this work is taken from the theory of quantum dissipation in open systems

$$J(\omega) = \omega^s f(\omega, \omega_c) \quad (4.19)$$

Where  $\omega_c$  is the characteristic frequency of the bath, and  $f(\omega, \omega_c)$  is a damping function which helps  $J(\omega)$  to vanish in the limit of  $\omega \rightarrow \infty$ . There are many different ways to choose  $f(\omega, \omega_c)$  (CITAR CITE From coherent motion to localization: II. Dynamics of the spin-boson model with sub-Ohmic spectral density at zero temperature), in this case we will choose an exponential cut-off damping type as  $f(\omega, \omega_c) = e^{-\omega/\omega_c}$ .

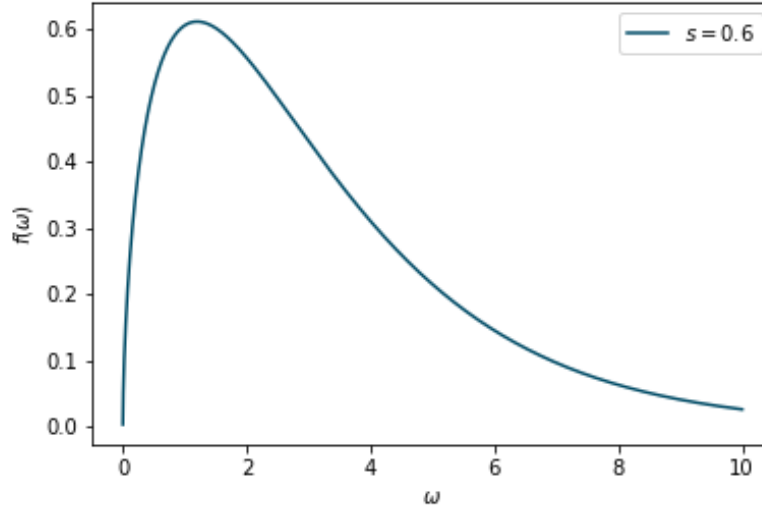


Figura 4.10: Frequency spectrum distribution without normalization for the case of  $s = 0,6$ .

### 4.3.2. Energy spectra

In this work we will monitor the energy spectra in two different ways, both are related to the idea of having a cloud of harmonic oscillators with initial conditions around the origin of phase space. The first idea is by drawing the energy of the oscillators from a distribution with a certain mean and variance, the second one consists of using the Box-Muller transform to sample a quasigaussian two dimensional distribution of harmonic oscillators in phase space.

#### 4.3.2.1. Drawing energy from a distribution

The method outlined in this subsection consists on drawing the energy of each harmonic oscillator from a probability distribution (mostly a gaussian) with a determined mean and variance. This method will let us normalize the energy of the heat bath at will, having the energy of each harmonic oscillator will let us compute the sum and divide each energy by the normalization desired.

Now to decide where to locate each oscillator we sample a random number from a uniform distribution  $[0, 2\pi)$ , this will represent an angle on a circle which will be deformed into an ellipse according to the energy and frequency of each harmonic oscillator obtaining finally a position of a harmonic oscillator according to a determined energy ellipse. This process is repeated for every oscillator on the bath giving as a result a distribution of oscillators in phase space with an energy distribution of the heat bath perfectly defined and normalized.

#### 4.3.2.2. Quasi-gaussian distribution in phase space

This method consists in implementing the Box-Muller transform algorithm onto a uniform distribution to obtain a two dimensional distribution grid of points that represent a gaussian with a defined mean and variance along each dimension (CITE CITAR BOX MULLER TRANSFORM).

### 4.4. Number of modes in the bath

A very important parameter to determine the dynamics of the system is the number of oscillators in the heat bath. According to dissipative dynamics theory, we retrieve an equation of Langevin type dynamics in the limit of infinite harmonic oscillators in the bath. We have already shown the behavior of the dynamics under the influence of only one harmonic oscillator coupled to the particle. What we will do in this work will be increase steadily the number of harmonic oscillators of a finite heat bath to achieve dissipative behavior without the need of extending the system to infinity. Therefore, it is important to keep an eye on the dynamics of each case of the number of harmonic oscillators and change different parameters of the system in order to understand in a more general way the behavior of the whole system as a function of the number of modes of the bath. This analysis will lead to the conclusion to modelate dissipative dynamics in a finite heat bath with a very small number of modes.

#### 4.4.1. Chaos to dissipation dynamics

In this section we will start to evidence the loss of chaotic dynamics due to the increasing number of oscillators.

#### 4.4.2. Variation of the double well and heat bath parameters

There are four types of parameters that are interesting for us to look at the variation of the dynamics of the system: The exponent  $s$  in the equation (4.19), the coupling constant of the oscillators  $g_0$  that multiplies the coupling constant of each oscillator  $g_i = g_0/\sqrt{N}$ , the height of the potential barrier and the initial energy of the heat bath. Each of these conditions will affect the number of jumps from one well to the other that the particle makes. We will therefore evaluate the results of changing these parameters for different number of oscillators for 100 test cases where the positions, frequencies and energies are randomized every time and the numbers of jumps will be averaged. The way of sampling the energies and initial conditions are described in the method of drawing energies from a gaussian distribution in order to have more control on the energies of the harmonic oscillators. For most of the cases we will use fixed values for each parameter unless explicitly stated otherwise, these values are  $s = 0,5$ ,  $g_0 = 0,1$ , the initial energy of the heat bath  $E_{bath} = 0,1$  and the height of the potential barrier  $PB = 1$

##### 4.4.2.1. Changing the exponent $s$

According to the microscopic theory of dissipation (CITAR CITE EL ARTICULO DE LEGGET), the exponent  $s$  in equation (4.19) controls the nature of the bath where  $s = 1$  is the “ohmic” case where it can be compared to a dissipative term proportional to velocity in the classical equation. The case of  $s > 1$  is called “super-ohmic” and the case of  $0 < s < 1$  is called “sub-ohmic”. Here we observe the behavior of the system in terms of the jumps between the wells seen for different numbers of harmonic oscillators and different values of the parameter  $s$ .

FIGURA FIGURE DE LOS SALTOS CAMBIANDO EL VALOR DE  $s$

We conclude that for the classical case, the parameter  $s$  in the spectral density does not really affect the dynamics of the system in a particular way as we don’t see a real difference between having a bath with sub-ohmic, ohmic or super-ohmic nature. We see the general behavior of dissipation where the jumps between the wells decrease with the increase in the number of oscillators in the heat bath and it is independent of the parameter  $s$ .

#### 4.4.2.2. Changing the individual coupling $g_0$

We have seen the effect of the coupling involving chaos with only one oscillator in one of the previous sections, this showed us the effect of different values for the coupling constants that develop into increasing chaotic motion. In this section we will continue to study the effects on the dynamics of the whole system when we use different values for the constant  $g_0$  that multiplies each of the individual coupling constants  $g_i \sim 1/\sqrt{N}$ . Previously, the method we used to describe the dynamics and the effects of the change in the coupling was the Poincaré surface section, with this method we could visualize the increase of chaotic dynamics when the rational tori got destroyed. Unfortunately, when we increase the number of harmonic oscillators, the Poincaré sections stop being very useful, this is due to the amount of degrees of freedom the system will have. We could visualize the dynamics of the system because there was only two degrees of freedom, this made it possible to find planes where the dynamics was projected and this were the Poincaré surface sections, when we increase the number of oscillators the Poincaré planes will become hyperplanes that we cannot visualize properly, this means we would have to project the planes onto lower dimensions but doing this we would lose most of the details of the dynamics. For this reason we will visualize the change of the behavior using the same method of analysing the frequency of jumps between the wells.

We simulated the dynamics of the 100 test cases for different values of  $g_0$  and different number of harmonic oscillators. We know from previous the experience of only one oscillator that if the coupling is strong the overall behavior will tend to be more chaotic, but now that we have more harmonic oscillators we start to see the effects of dissipation over chaos. A big coupling constant will continue to result in strong interactions between the oscillators and the particles, but the tendency of the particle to stay on one side will prevail.

FIGURA FIGURE DE LOS SALTOS CAMBIANDO EL VALOR DE  $G$

In Figure (REFERENCIAR LA FIGURA ANTERIOR) we evidence that the overall tendency of dissipation is observed when the number of harmonic oscillators increases regardless the coupling constant  $g_0$  (for  $g = 0,001$  in the figure we believe for a bigger number of harmonic oscillators this behavior will be seen). It is also interesting to see that for coupling  $g_0 = 0,3$  the curve descends really fast but seems to start to grow again, this can be attributed to the fact that this value for the coupling constant starts to be a very strong interaction of the bath with the system making it not very suitable for a dissipation model in long term.

#### 4.4.2.3. Changing the initial energy of the heat bath

The initial energy of the heat bath is an important parameter statistically speaking, this is because it represents the “temperature” of the environment our central system is located in.

If the whole system has initially a very high temperature then the dynamics will become very difficult to predict in long term as it will take longer time to reach a thermal equilibrium, if we take the temperature of the system to be relatively low compared to the height of the unstable equilibrium point where the particle is always located then we can see how energy from the particle is transferred to the heat bath in a somewhat irreversible manner. This analysis involved then different initial energies for the heat bath and how it affects the number of jumps between the wells of the particle.

FIGURA FIGURE DE LOS SALTOS CAMBIANDO EL VALOR DE  $E_{bath}$

In Figure (REFERENCIAR LA FIGURA QUE ACABO DE HACER) we can evidence that the different initial energies of the heat bath will result in a change of scale of the number of jumps that the particle suffers. The overall behavior of dissipation is continued to be present. For a heat bath with a high initial energy or “temperature” we see that the particle jumps between the wells more times than for a small energy but when the number of oscillators increases then the jumps decrease. When we “freeze” the heat bath by giving it a low initial energy we experience less jumps between the wells and a faster decay of it when the number of oscillators increase. Then we can conclude that the overall consequence of changing the initial energy of the heat bath will be a scaling factor in the exponential decay of the jumps.

#### 4.4.2.4. Changing the height of the potential barrier

The particle of the central system is located on the unstable equilibrium unless otherwise stated for the simulations done in this work, then a very interesting parameter to study is the difference in the dynamics when this unstable equilibrium point located on the top of the potential barrier is changed. We recall that the shape of the quartic potential for the particle is given by equation (4.9) where the parameters  $a$  and  $b$  are in charge of the shape of the double well potential. We have shown previously in equation (4.18) that the height of the potential barrier is completely determined by the parameters  $a$  and  $b$  and that the resonance frequency of small oscillations for the two minima is given by equation (4.13) which only depends on parameter  $a$ . This ideas are relevant to determine how to change the potential barrier height, if we change  $a$  and  $b$  but maintaining the ration  $a/b$  we will rescale the whole potential, but this is not considered because this means that the resonance frequency will change and the particle will have to travel more distance to imitate the same kind of dynamics as before meaning it will require more calculation time. The way we changed the height is by only changing the parameter  $b$ , this will maintain



## APPROACH TO THE MEASUREMENT THEORY

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### 5.1. Classical Measurement

#### 5.1.1. Stability of a system

### 5.2. Quantum Measurement

#### 5.2.1. Postulates of Quantum Mechanics

### 5.3. Can this be considered as a measurement?





## RELATED WORK

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### 6.1. Quantum measurement in a unitary setting



## FUTURE WORK

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## CONCLUSION

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## APÉNDICE A

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### EXTRA INFORMATION

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Some more text ...

