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Chaos in Constrained Systems

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DECLARATION

This thesis was written in the Department of Mathematics, University of Ghana, Legon and Perimeter Institute for Theoretical Physics, Waterloo, Canada from September 2014 to July 2015 in partial fulfilment of the requirement for the award of Master of Philosophy degree in Mathematical Physics under the supervision of Dr. Philipp Höhn of the Perimeter Institute for Theoretical Physics.

I hereby declare that except where due acknowledgement is made, this work has never been presented wholly or in part for the award of a degree at the University of Ghana or any other University.

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Abstract

Chaos poses technical challenges to constrained Hamiltonian systems. This is an important topic for discussion, because general relativity in its Hamiltonian formulation is a constrained system, and there is strong evidence that it exhibits chaotic features. We review concepts in gauge systems and their association with Hamiltonian constraints, relational Dirac observables as gauge invariant encodings of physical information, and chaos in unconstrained Hamiltonian systems. We then construct a non-integrable, ergodic toy model, and with it explicitly illustrate the non-existence of a maximal set of Dirac observables, and a solution space which fails to be a manifold. The potential consequences of these qualitative features of a chaotic constrained Hamiltonian system for general relativity and the quest for its quantum theory are deliberated.

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Chapter 1

Introduction

Constraints arise when physical theories with gauge degrees of freedom are cast in the Hamiltonian formulation [12, 16]. A class of these constraints act as generators of gauge transformations, which introduce a degree of arbitrariness in the theory's specification of the physical state of the system [12, 16]. A physical state is not uniquely represented by a point in phase space, where Hamiltonian dynamics is described, but by a continuum of points known as the gauge orbit, which are connected by gauge-transformations.

The challenge arises to encode the true physical state of the system in a way which is invariant under these gauge transformations. In some theories such as Yang-Mills theory and quantum electrodynamics, it is possible to do this, because the Hamiltonian is a true Hamiltonian which generates time evolution. One can obtain the needed physical information by an appropriate gauge-fixing procedure, which specifies a unique point on each gauge orbit with which the theory is described. This is not always globally possible, but locally (in configuration space) this can be done. Although one can perform gauge fixings in these cases, in order to construct a quantum theory, one usually considers a path-integral quantization as it turns out to be more convenient [26].

Einstein's general relativity is qualitatively different from the theories mentioned above. One can also cast general relativity into a Hamiltonian formulation [3, 8]. There one finds a Hamiltonian constraint: the Hamiltonian comprises only a sum of constraints which generate gauge transformations, and the dynamics in terms of a refoliation with spatial hypersurfaces in spacetime. The symmetry generated by the Hamiltonian constraint is the refoliation invariance of a general relativistic spacetime. No 'true' Hamiltonian that generates 'time evolution' in the usual sense of a background time.

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Because of this nature of general relativity, two issues need to be addressed. The first is to find a suitable way to encode only the physically relevant information in the theory. Dirac observables, in principle, achieve this goal. These are global, smooth functions on the constraint surface which are constant on gauge orbits, which means they have the property that they do not change along the gauge orbit that corresponds to a physical state. If sufficiently many independent of such quantities can be constructed, they are useful for characterizing the distinct physical states of the theory. Additionally, it is possible to construct a space smaller than the original phase space, on which each point corresponds to a separate physical state or trajectory. This is known as the reduced phase space. If there are enough independent Dirac observables and this space is defined, the Dirac observables satisfy a Poisson algebgra on the reduced phase space similar to that of which is satisfied by phase space variables in an unconstrained Hamiltonian system [16]. Because of this property, if the reduced phase space exists, and there is an algebra of Dirac observables on it, one would have a way of representing only physically relevant information.

The second issue that needs to be addressed is the concept of time evolution. Before special and general relativity, time played a privileged role in the description of the dynamics of systems. In general relativity, time itself is a part of the dynamical aspects of the theory. There is no notion of absolute, external time, independent of all other quantities, and on which the rest of the theory depends. An approach to dealing with this is to consider relational dynamics, which correlates the values of physical quantities to those of other physical quantities, the latter chosen to serve as 'clocks' [9, 13, 17, 27]. The idea behind this is not completely special: indeed, physics is mostly carried out by relating quantities. For instance, in considering the motion of a car, one reads the position of the car at a certain time. This forms the basis of the description of the dynamics, out of which concepts such as velocity and acceleration are derived. The key difference is that time in general relativity is observer-dependent, and the theory is formulated to take this into account, without biasing towards a particular perspective. Consequently, one seeks in relational dynamics to relate physical quantities in the theory in appropriate ways, in order to extract a notion of dynamics out of the theory.

In order to construct Dirac observables and specify relational dynamics however, one needs the complete set of solutions to the equations of motion [16]. One could possibly encounter a problem doing this, and that is the main motivation for this thesis. In particular, in general relativity it seems hopeless to solve the Einstein equations in full generality. In the case of dynamical systems which are

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non-integrable and may feature chaos, one cannot solve the system completely. Consequently, one cannot construct global, smooth Dirac observables, or global, smooth prescriptions to the relational dynamics. This is important to consider, because there is strong evidence for chaotic behaviour in general relativistic systems.

Indeed, Newton's gravitational theory exhibits chaotic dynamics for systems with greater than three bodies [2]. General relativity is a much more sophisticated theory, which reproduces Newton's mechanics in the appropriate limit, so one does not expect an improvement of the situation.

Additionally, some solutions of general relativity have been shown to possess chaotic features. The Friedmann-Robertson-Walker (closed with a minimally coupled massive scalar field) universe, which is one of the simplest solutions to general relativity, possesses chaotic dynamics. Cornish et al [10] compute the topological entropy of this model and show that it is non-zero. In addition, they give numerical evidence of a fractal structure on the initial data (which characterizes the solutions, and gives evidence for a lack of a reduced phase space manifold). There also exists some analytic evidence that there is a fractal structure in the solution space [5, 19, 25].

Another solution to general relativity that displays chaotic behaviour is the Mixmaster universe introduced by Misner [22]. This model has also been shown to be chaotic [11, 23].

Additionally, the Belinsky-Khalatnikov-Lifshitz (BKL) conjecture posits that generic cosmological solutions to the Einstein field equations feature chaotic behaviour [6].

In chaotic systems, relational Dirac observables cannot be constructed globally, and there is no reduced phase space endowed with a Poisson algebra on which the physically meaningful information in the theory can be encoded.

The above discussion is in turn important for some approaches to constructing a quantum theory of gravity. Specifically, these are the canonical quantum gravity approaches, based on the prescription of canonical quantization originally invented by Dirac [8, 27, 32]. For a general classical theory, quantization may follow one of two approaches. One of these is reduced phase space quantization, which constructs the reduced space which contains only physical information as briefly mentioned, and then quantizes it. But this is a hopeless approach as far as general relativity is concerned. The other is Dirac quantization, which first quantizes the theory without removing the non-physical degrees of freedom, and then solves the constraints in the quantum theory to construct the physically meaningful states.

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This thesis begins with a review of relevant ideas, and culminates in the consideration of a chaotic model in which we show that a reduced phase space does not exist for this model. This straightaway rules out reduced phase space quantization. While Dirac quantization is possible to carry out in principle, there arises the conceptual question of how the observables one obtains in the quantum theory relate to the physical degrees of freedom of the original classical theory.

1.0.1 Scope of the thesis

The thesis is organized in three main parts. Sections 2 through 4 are the review part of the thesis, and discuss some important relevant concepts. Section 5 constitutes the main research part of the thesis, and section 6 concludes.

Section 2 In this section, the realization of constraints in theories with gauge degrees of freedom, and the manner in which a class of them generate gauge transformations, is reviewed.

Section 3 In this section, the problem of extracting physically relevant information is addressed, and we discuss relational dynamics. We also give a short discussion on the reduced phase space with its algebra of Dirac observables, and how this encodes the physical information of a theory.

Section 4 This section is a review of chaos in unconstrained Hamiltonian systems. Concepts that are important to understanding the potential role of chaos in constrained systems are discussed. Section 4 concludes the review part of the thesis.

Section 5 In section 5, we construct a model in which we explicitly show the non-existence of an algebra of Dirac observables and a reduced phase space. Section 5 is the main research part of the thesis.

Section 6 Finally, in the last section we give a brief review of the contents of the thesis before, and deliberate on the importance of the issues addressed in this thesis to the larger picture of the physics of general relativity and the quest for its quantum theory.

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Chapter 2

Canonical analysis, constraints, and gauge systems

In this section, we discuss the Hamiltonian formulation of dynamics, and how constraints show up in systems with gauge degrees of freedom. The discussion of this section is mainly a review of well-known literature, primarily from those authored by Dirac [12] and Henneaux and Teitelboim [16].

As in the standard Lagrangian formulation of physics, one proceeds by the principle of least action. The theory is specified in terms of positions q_n, $n = 1, \cdots, N$ for N physical degrees of freedom, and their velocities $\dot{q}_n = \frac{dq_n}{dt}$. One can generalize this to infinitely many degrees of freedom for a field theory, but that will not be required for this thesis. The variables $(q, \dot{q})$ specify the *configuration space* of the theory. There is an action integral

$$S = \int_{t_1}^{t_2} L\,dt. \tag{2.1}$$

dependent on the physical system, which when varied and conditioned to be stationary, with fixed limits of integration (corresponding to the end points of the trajectory of the system), one obtains the equations of motion

$$\frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}_n}\right) = \frac{\partial L}{\partial q_n}\,. \tag{2.2}$$

The quantity $L(q, \dot{q})$ is the *Lagrangian*. An important reason why one generally begins with the action integral is that correspondence with the required symmetries of the theory is manifest. If the Lagrangian one writes down is invariant under symmetry transformations, then the resulting equations of motion obey the

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required symmetries.

Given sufficiently many initial conditions, one can attempt to solve the equations of motion (2.2) to specify the dynamics of the system for all time. Whether that is possible will be an important topic for discussion in this thesis, as we will see later on.

The Hamiltonian formulation, in terms of (q, p) variables, is obtained via a Legendre transformation from the Lagrangian description in terms of $(q, \dot{q})$ variables. The p variables are the momenta, defined by

$$p_n(q, \dot{q}) = \frac{\partial L(q, \dot{q})}{\partial \dot{q}_n}. \tag{2.3}$$

This definition can be used to map $(q, \dot{q})$ variables to (q, p) variables. In some cases, the map in equation (2.3) is invertible. If that is so, the momenta, written explicitly as functions of q_n and $\dot{q}_n$, may be inverted to obtain the velocities $\dot{q}_n = (q_n, p_n)$ as functions of the positions and the momenta. In general, the momenta-defining maps are not invertible. This will have an important consequence, as will be seen shortly. If the map that defines the momenta is singular (non-invertible), then by the implicit function theorem, there will be relations between the positions and momenta that can be arranged into the form $\phi_i(q, p) = 0$, $i = 1, \cdots, M$, where i is an index that labels the M independent relations of this type. In other words, not all of the variables in (q, p) space are dynamically independent. The relations $\phi_i(q, p) = 0$ define a subset of phase space to which the dynamics is constrained. These relations will be termed *primary constraints*.

Further, the Hamiltonian defined in the usual way via $H(q, p) = p_n\dot{q}_n - L$, is a quantity that can be expressed in terms of positions and momenta, independent of velocities. The Hamiltonian is a function of phase space variables that is constant on the trajectories of the system, in the case of time-independent Hamiltonians. This property uniquely specifies how the system must evolve in phase space for all time, given a set of initial data (q, p). If there are constraints in the theory, then as mentioned previously, not all of phase space is accessible. For the theory to be consistent, phase space variables must always be found on the constraint surface. When constraints arise, the Hamiltonian is not uniquely defined as a function of the phase space variables. This is because for consistent equations of motion, the phase space variables should always lie on the constraint surface. However, on this surface, the constraints $\phi_i(q, p)$ vanish such that we could add an arbitrary linear combination of constraints to the Hamiltonian. Thus we write

$$H^* = H + c_i\phi_i, \tag{2.4}$$

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where the c_i's are arbitrary coefficients which act as Lagrange multipliers and can in general be any function of phase space, without changing the theory. The phase space variables q and p can be varied independently only so long as they satisfy all the primary constraint relations. The equations of motion, obtained via variational methods, are:

$$\dot{q}_n = \frac{\partial H}{\partial q_n} + u_m \frac{\partial \phi_m}{\partial p_n} \tag{2.5}$$

$$\dot{p}_n = -\frac{\partial H}{\partial q_n} - u_m \frac{\partial \phi_m}{\partial q_n}\,, \tag{2.6}$$

where u_m are unknown coefficients that need to be determined.

2.0.1 Poisson Brackets, dynamics and gauge transformations

The equations of motion can be conveniently written using Poisson brackets, which are defined as follows: for any two functions on phase space $f(q,p)$ and $g(q,p)$, the Poission bracket between f and g is:

$$\{f,g\} = \frac{\partial f}{\partial q_n}\frac{\partial g}{\partial p_n} - \frac{\partial f}{\partial p_n}\frac{\partial g}{\partial q_n}\,. \tag{2.7}$$

A number of properties follow from the definition of the Poisson brackets. They are anti-symmetric in their arguments, linear in both arguments, obey the ordinary product rule of differentiation and obey the Jacobi identity

$$\{A,\{B,C\}\} + \{B,\{C,A\}\} + \{C,\{A,B\}\} = 0\,. \tag{2.8}$$

Using this definition, we can write for any phase space function

$$\dot{g} = \frac{\partial g}{\partial q_n}\dot{q_n} + \frac{\partial g}{\partial p_n}\dot{p_n}\,. \tag{2.9}$$

Substituting in the expressions for $\dot{q_n}$ and $\dot{p_n}$ from the equations of motion allows us to write:

$$\dot{g} = \{g,H\} + u_m\{g,\phi_m\}\,. \tag{2.10}$$

Here we observe that an extra term appears which does not arise in the usual case of unconstrained Hamiltonian mechanics.

The Poisson bracket structure is only defined for differentiable functions of the q's

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and the p's. We could write down the expression:

$$\dot{g} = \{g, H + u_m\phi_m\}\,, \tag{2.11}$$

and note that this is not well defined, because the u_m's can be solved for as functions of $(q, \dot{q})$, using equations (2.3) and (2.5). However, ignoring that problem momentarily, and computing the expressions using linearity and the product rule, we obtain:

$$\dot{g} = \{g, H\} + u_m\{g, \phi_m\} + \phi_m\{g, u_m\}\,. \tag{2.12}$$

The Poisson brackets in the first and second terms are well defined, but not those in the last terms. However, we can use the fact that ϕ_m vanishes for consistent equations of motion to obtain the well defined expression:

$$\dot{g} = \{g, H + u_m\phi_m\} = \{g, H\} + u_m\{g, \phi_m\}\,. \tag{2.13}$$

It is important to note that the Poisson brackets are worked out before the fact that $\phi_m(q,p) = 0$ is used. This amounts to working out the form of the expression and then invoking the condition that the theory is restricted to a subspace of phase space. Hereafter, we will use the notion of *weak equality* to keep track of this rule. Two functions on phase space are said to be weakly equal if they differ only off the constraint surface. The symbol '$\approx$' is used[1]. If we take the constraints $\phi_i(q,p)$ to be functions on the entire phase space, then by their definition we write:

$$\phi_i(q,p) \approx 0\,. \tag{2.14}$$

It follows from the definition also that if two functions F and G are weakly equal ($F \approx G$), then their difference must be some combination of all the constraints, i.e.

$$F - G = c_i(q,p)\phi_i(q,p)\,. \tag{2.15}$$

The above expression is true because by construction, the constraints are the only independent functions that vanish on the constraint surface. If two functions are equal everywhere on phase space, we say they are *strongly equal*, and use the regular symbol '$=$'. With all of this is mind, one can more concisely write:

$$\dot{g} \approx \{g, H + u_m\phi_m\}\,, \tag{2.16}$$

as the equation of motion of a phase space function g, and then define the *total*

[1]Weak equality is defined with respect to a set of constraints. As we will see, other constraints can arise, and what constitutes weak equality needs to be modified.

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Hamiltonian to be:

$$H_T = H + u_m \phi_m \,. \tag{2.17}$$

As mentioned earlier, for consistency in the construction, phase space variables must always lie on the constraint surface. The constraints themselves, which define this surface, are functions on space phase. We should require that at all times, $\phi_i \approx 0$. Since ϕ_i is itself a function of q and p, we may compute what $\dot{\phi}_i$ is just as we would for any phase space function, and demand that the right hand side of the equation

$$\dot{\phi} = \{\phi_m, H\} + u_{m'}\{\phi_m, \phi_{m'}\} \tag{2.18}$$

vanish for solutions for consistency. We could compute this expression and obtain one of a number of different possible outcomes.

- Inconsistent system: The first possibility is that it would lead directly to an inconsistency. This is not a very interesting case, as it tells us immediately that the Lagrangian we started off with did not make much sense (this would be the case for instance, if we took $L = q$ and evaluated the equations of motion).

- Trivially consistent: The second possibility is that the right hand side automatically vanishes.

- Secondary constraints: Another is that it reduces to an equation independent of the u's. This particular case can be written as an expression similar to what defined the primary constraints. We write them as $\chi(q, p) = 0$ and call them *secondary constraints*. Eventually, distinguishing between 'primary' and 'secondary' constraints will not be very important, as another classification of the constraints will be seen to be of more practical importance. See Dirac [12] and Henneaux and Teitelboim [16] for further discussion on the classification of constraints.

- Fixed u's: The last possibility is that it imposes conditions that the u's must satisfy, so that they become quantities fixed in a particular way. Note that this requires $\{\phi_m, \phi_n\} \not\approx 0$ for at lease some pair m, n.

Just as one will demand consistency for the primary constraints, the χ's themselves must satisfy $\dot{\chi} \approx 0$. We can work out what this equation leads to. If they lead to a new set of constraints, those will be termed *tertiary* constraints, and the same consistency conditions will be required of them. The process of requiring consistency in any constraint that arises continues until we end at a self-consistent set of relations. At that point, one would have a set of primary constraints, a set of secondary constraints, tertiary constraints (arising from secondary constraints, and so on), and a number of conditions on the u_m coefficients.

Going back to the point of the difference between primary and secondary constraints (this also is true of tertiary, and so on) not being of much practical importance in the setup of the theory, we at this point clump all the constraints together into one set and index them with the same letter. So that we write:

$$\phi_j \approx 0; \quad j = 1, \cdots, W, \tag{2.19}$$

where W is the total number of constraints that arise until a self-consistent condition is met. The next step is to deal with the set of relations that impose conditions on the u's that we mentioned, which are of the form:

$$\{\phi_j, H\} + u_m\{\phi_j, \phi_m\} \approx 0\,. \tag{2.20}$$

We could solve for some the u's as $u_m = u_m(q,p)$ by viewing the conditions as a set of inhomogeneous equations. The most general solution will be a linear combination of the particular solution to the equation, which we term $U_m(q,p)$, and any arbitrary linear combination of the solution to the associated homogeneous equation $u_m\{\phi_j, \phi_m\} \approx 0$, which we write as $v_a V_{am}$. The v_a's are arbitrary coefficients, and the V_{am}'s are the independent solutions to the homogeneous equation, labelled by a for as many as there are, and m for the particular u_m to which they are associated. Hence we have:

$$u_m = U_m + v_a V_{am}\,, \tag{2.21}$$

and going back to the definition of the total Hamiltonian, we have:

$$H_T = H + U_m\phi_m + v_a V_{am}\phi_m\,. \tag{2.22}$$

To make things a bit neater, we write:

$$H_T = H' + v_a\phi_a; \quad \phi_a = V_{am}\phi_m; \quad H' = H + U_m\phi_m\,. \tag{2.23}$$

The take away point at the present moment is that after demanding consistency in the theory, one still has v_a's which are completely arbitrary. These give an indication as to what the nature of the present theory is. Because the Hamiltonian contains arbitrary coefficients, which can themselves be time-dependent functions, dynamical variables in future times are not completely determined by

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initial conditions (this will be seen in more detail in equation (2.27) below).

We will now return to the point of classifying the constraints. As mentioned earlier, distinguishing between constraints as primary or secondary (or tertiary etc.) is not of much importance. The difference arises due to the nature in which they first appeared in the theory, beginning with the Lagrangian, passing on to the Hamiltonian, and then requiring consistency. Beyond that, they should be treated on the same footing. Instead we will give the following definition: a function $F(q,p)$, on phase space is said to be *first class* if it satisfies the following condition[2]

$$\{F, \phi_j\} \approx 0 \ \ \forall j \, . \tag{2.24}$$

F is otherwise second class. If F is first class, then any $\{F, \phi_j\}$ must strongly equal a linear combination of the ϕ's, so that:

$$\{F, \phi_j\} = r_{jj'} \phi_{j'} . \tag{2.25}$$

An important fact to note is that the Poisson bracket of two first class functions is also first class. This is straightforward to show by evaluating $\{\{F, R\}, \phi_j\}$, for first class phase space functions F and R, using the Jacobi identity and the fact that F and R are first class. From equation (2.8) we have:

$$\begin{aligned}
\{\{F, R\}, \phi_j\} &= \{\{R, \phi_j\}, F\} - \{\{F, \phi_j\}, R\} \\
&= \{r_{jj'} \phi_{j'}, F\} - \{f_{jj'} \phi_{j'}, R\} \\
&= r_{jj'} \{\phi_{j'}, F\} + \phi_{j'} \{r_{jj'}, F\} - f_{jj'} \{\phi_{j'}, R\} - \phi_{j'} \{f_{jj'}, R\} .
\end{aligned} \tag{2.26}$$

The first and third terms in the last expression must vanish because F and R are first class phase space functions. The remaining terms vanish for consistent equations of motion because $\phi_{j'}$ is a constraint. Hence, $\{F, R\}$ is first class, if F and R are both first class. This fact will be important shortly.

The constraints themselves are phase space functions, and can be classified as first class and second class using the above definitions. Also, the quantities $H' = H + U_m \phi_m$ and $\phi_a = V_{am} \phi_m$ which have been defined earlier are also first class phase space functions. Hence, the Hamiltonian is a sum of first class quantities. The index a runs over all the independent arbitrary functions of time occurring in the general solution to the theory (the arbitrary functions arise as the coefficients to the homogeneous parts of the solutions to the equations which fix the u_m's). Arbitrary functions of time correspond to gauge degrees of freedom in a physical

[2] As more constraints have arisen, the weak equality used in equation (2.24) takes all of the W constraints in equation (2.19) into account.

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theory. If one were to start from some physical state and evolve it in time, there is not a unique state that one could reach in the theory. How this arises will be discussed shortly. Consequently, any point on phase space does not represent a unique description of the system. Some other state on phase space could have been reached by choosing the arbitrary functions differently, for the same initial data, but these must be physically equivalent. Hence, each physical state is described by a continuum of points on the constraint surface.

Gauge degrees of freedom arise in theories that encode the ability to make certain arbitrary changes to quantities in the theory. This is the case in General Relativity, which must account for the freedom to make local coordinate transformations without altering the equations that describe the physics. General Relativity is a constrained Hamiltonian system. The Hamiltonian consists only of constraints, and no true Hamiltonian that generates dynamics [3, 8].

Let us now make the discussion more explicit. These transformations, called *gauge transformations* in the theory can be inspected infinitesimally. As pointed out above, all points on phase space that evolved from the same initial state must correspond to the same physical state. Consider some initial value of a phase space function, $g_0 = g(0)$. Its value after an infinitesimally short time is:

$$\begin{aligned} g(\delta t) &= g_0 + \dot{g}\delta t \\ &= g_0 + \{g, H_T\}\delta t \\ &= g_0 + \delta t[\{g, H'\} + v_a\{g, \phi_a\}]. \end{aligned} \tag{2.27}$$

Suppose we chose different values of the coefficients v, say v' (the entire point here is that we are free to do so). Then we may write the difference between the new and the old g as:

$$\Delta g(\delta t) = \delta t(v_a - v'_a)\{g, \phi_a\}, \tag{2.28}$$

which can be re-written as:

$$\Delta g(\delta t) = \epsilon_a\{g, \phi_a\} \qquad\qquad \epsilon = \delta t(v_a - v'_a)\,, \tag{2.29}$$

so that ϵ_a is some small arbitrary number that is determined by the choice of v's. Any function g may be changed by an amount $\Delta g(\delta t)$ defined above (in particular, the phase space function could be the phase space coordinates (q_n, p_n) themselves), and this should correspond to the same physical state. In essence, we use $\epsilon_a\phi_a$ as generators of local transformations that do not affect the physical sate.

The conclusion here is that the first class constraints generates gauge transformations in the theory. This is because the first class constraints are the part of the

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Hamiltonian that are contracted with arbitrary functions, which induces arbitrariness in the description of a physical state. Given a point on the constraint surface, a set of points can be reached from this point using these gauge transformations. This set of points is termed the *gauge orbit*. This is the continuum of points that was earlier mentioned, and all points on phase space belonging to a gauge orbit correspond to the same physical state. Thus a physical state is not represented by a point on the constraint surface, but a whole continuum of points, the gauge orbit. There will be many of such gauge orbits, and each one of then corresponds to a distinct physical state of the theory.

Using the fact mentioned earlier that the Poisson bracket between two first class quantities is also a first class quantity, the first class constraints generate an algebra, by taking Poisson brackets between them, which is closed under the requirement that the result of this operation be a first class quantity. This resulting quantity can itself be used to generate gauge transformations in the same manner as described above. Taking this into account, the final step in the present section is to define the extended Hamiltonian

$$H_E = H_T + v'_{a'}\phi_{a'}, \tag{2.30}$$

by adding all the possible generators of gauge transformations. The index a' runs over the full list of first class constraints, those that we termed primary constraints, as well as all those that are obtained by taking Poisson brackets of constraints with each other and demanding that they vanish for consistent equations of motion.

The discussion can be extended to the field theories. This will not be required for this thesis. For a detailed discussion, see Henneaux and Teitelboim [16] and Bojowald [8].

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Chapter 3

Observables in constrained systems

In the previous section, we have seen that constraints not only restrict the accessible parts of phase space in the theory, but they constitute generators of gauge transformations if they are first class. These transformations generate a subset of the constraint surface that must be identified with a physical state. This section discusses ways in which one can construct quantities that encode the physically relevant information in the theory. Since an entire gauge orbit is identified with a physical state, such quantities must take the same value everywhere on the gauge orbit. These will be called the observables of the theory. If there are enough independent such quantities, we can parametrize distinct physical states in the solutions of the system.

Before doing this, some mathematical preliminaries are discussed to express ideas in the previous section slightly more formally, and introduce a few new concepts. Still following the scheme of using a theory with a finite number of degrees of freedom, phase space will be a $2N$-dimensional manifold (for a theory with N finite degrees of freedom) with co-ordinates $x = (q^i, p_i)$ and symplectic structure $\{q^i, p_j\} = \delta^i_j$. Also, suppose that there are some $J \leq N$ first class constraints $\{\phi_j\}_{j=1}^{J}$ which generate an algebra with respect to taking Poisson brackets between them that can be written as

$$\{\phi_i, \phi_j\} = f_{ij}{}^{k}\phi_k. \tag{3.1}$$

Hereafter we will relabel the constraints as $C_i := \phi_i$.

The symplectic structure allows us to associate any phase space function, F, with a vector field χ_F, by defining

$$\chi_F \cdot f := \{f, F\}, \tag{3.2}$$

where $\chi_F \cdot f$ denotes the action of the vector field χ_F on an arbitrary phase space function, f. Written in phase space coordinates $\{x_i\}_{i=1}^{2N}$, the action of the vector field is

$$\chi_F \cdot f := (\chi_F(x))^i \frac{\partial}{\partial x_i} f(x), \tag{3.3}$$

where $(\chi_F(x))^i$ are the components of $\chi_F(x)$ in the given coordinate system.

The function F generates a flow $\alpha_F^t(x)$,

$$\alpha_F^t(x) : \mathcal{P} \to \mathcal{P}\,, \tag{3.4}$$

$$x \mapsto \alpha_F^t(x), \tag{3.5}$$

on phase space $\mathcal{P}$, with flow parameter t. The map $\alpha_F^t(x)$ is defined as the solution to the equation

$$\frac{d}{dt}\alpha_F^t(x) = \chi_F \cdot \alpha_F^t(x). \tag{3.6}$$

That is, the vector field χ_F is tangent to the flow lines. By varying t continuously, the image of a point x under $\alpha_F^t(x)$ varies smoothly, so that for a given point x_0, $\alpha_F^t(x_0)$ defines a curve on phase space parametrized by t

$$\alpha_F^t(x_0) : \mathbb{R} \to \mathcal{P} \tag{3.7}$$

$$t \mapsto \alpha_F^t(x_0). \tag{3.8}$$

Using the flow generated on the phase space point, one could also define the action of the flow on a phase space function $f \in C^\infty(\mathcal{P})$, where $C^\infty(\mathcal{P})$ is the set of smooth functions on phase space, as a map $C^\infty \to C^\infty$ so that

$$f \mapsto \alpha_F^t(f) \tag{3.9}$$

$$\alpha_F^t(f)(x) := f(\alpha_F^t(x)) \tag{3.10}$$

where the second equation above defines the map in the first line. This simply means that one takes the value of the function f at the point $\alpha_F^t(x)$ which the point x moves to under the flow. One can write a formal expression for the flow on a function as [14]:

$$\alpha_F^t(f)(x) = \sum_{n=0}^{\infty} \frac{t^n}{n!} \{f(x), F(x)\}_{(n)} \,. \tag{3.11}$$

The notation used in the expression with the Poisson brackets refers to nested Poisson brackets, which are defined via

$$\{f, \cdot\}_{(0)} := f \tag{3.12}$$

$$\{f, \cdot\}_{(n)} := \{\{f, \cdot\}_{(n-1)}, \cdot\}, \tag{3.13}$$

so that the nested Poisson brackets give higher order derivatives, and the formal expression is similar to a Taylor expansion. Given that $\alpha_F^t(f)$ is a flow, it must satisfy,

$$\alpha_F^t(f) \circ \alpha_F^s(f) = \alpha_F^{t+s}(f). \tag{3.14}$$

We shall call the submanifold of phase space where all the constraints vanish the constraint hypersurface and denote it by $\mathcal{C}$.

Using the above definitions, gauge transformations take the following form: for a first class algebra of constraints, a gauge transformation G, is a map on the constraint surface $\mathcal{C}$ defined by

$$G(x) := \alpha_{\beta_i C_i}(x) := \alpha^1_{\beta_i C_i}(x) \tag{3.15}$$

for a set of real parameters $\{\beta_i\}_{i=1}^J$. This is a map from the constraint surface to itself because of equation (3.1). Since the constraints commute on the constraint surface, they will preserve each other. The meaning of the expression in equation (3.15) is as follows: the gauge transformation $G(x)$ of a point x is obtained via a composition of the flows generated using the constraints C_i. The time parameter in each of the flows is set to $t = 1$, and the parameters β_i are used to scale the constraints to determine how far along each flow one moves. If the the constraints do not all commute off the constraint surface, one has a non-abelian gauge theory. In abelian gauge theories, all the constraints commute both on and off the constraint surface, so that for all gauge transformations, the ordering of the composition does not matter. This last point will not matter in this thesis, as the specific examples looked at have only one constraint, and are thus trivially abelian.

Acting with the flows of the constraints on a point on the constraint surface generates an J-dimensional submanifold of $\mathcal{C}$. This submanifold is the gauge orbit.

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So far, we have established that all points on a gauge orbit on the constraint surface must correspond to the same physical state. In particular, all phase space states that evolve from the same initial physical state, but differ only due to the flow generated by the constraint with different choices of the arbitrary functions, must correspond to the same physical state.

We would like to formulate some gauge invariant quantity to encode only the physically relevant information of the theory. The so-called *Dirac observables* achieve this objective. A Dirac observable is a global, smooth function[1] on the constraint surface that satisfies the property:

$$\{O, C_i\} \approx 0, \tag{3.16}$$

for all the first class constraints $\{C_i\}$[2]. Thus, Dirac observables are invariant under the flow generated by the constraints: they are gauge invariant. A maximal independent set of Dirac observables parametrizes the distinct physical states of the system.

3.0.1 Complete observables as gauge invariant quantities

We discuss one scheme for determining the Dirac observables. These are *complete observables*, which are constructed from *partial observables*. The ideas here were first discussed by Rovelli [27] for the case of one constraint, and later extended to the case of many constraints by Dittrich [13].

The scheme begins by choosing a set of J algebraically independent phase space functions $T^k(x)$. These will be called the 'clock variables' and will be used to parametrize gauge orbits. The clock variables are chosen so that for every one of the constraints C_i, there is a unique clock variable that satisfies $\{T^i(x), C_i\} \not\approx 0$ and commutes with all the other constraints. $T^k(x)$ will have some fixed values τ^k that fulfils the condition that $T^k(x) = \tau^k$ on only one point on each gauge orbit. The choice needs to satisfy the conditions that

1. The gauge fixing must be accessible, that is, for any point x on the gauge orbit, there must exist a gauge transformation that maps x onto a point y that satisfies the gauge-fixing condition $T^k(y) = \tau^k$ and
2. $T^k(y) = \tau^k$, for $k = 1, \cdots, J$ must fix the gauge completely.

[1]Throughout the text so far, whenever a phase space function has been mentioned, we have implicitly assumed that it is smooth everywhere, thus infinitely many continuous derivatives may be taken.

[2]The index i here runs over all the independent first class constraints.

These conditions cannot in general be reached in most interesting cases in physics. Non-abelian gauge theories prove challenging, and the case of general relativity is not fully understood. For certain solutions, this is not possible [35].

In order to construct the needed observable quantities, we shall introduce some ideas that are important in gauge theories, and illustrate them with a single particle with one degree of freedom q. Consider a theory of a single particle, with one degree of freedom, q. The action integral is

$$S = \int_{t_1}^{t_2} dt\, L(t, q(t), \dot{q}(t)). \tag{3.17}$$

We can introduce an artificial 'time' parameter s to reparametrize the dynamics and render the Newtonian time t into a dynamical variable[3]. Namely, he action is redefined as the extended action

$$\begin{aligned} S_{ext} &= \int_{s_1}^{s_2} ds\, L\left(t(s), q(s), \frac{q'(s)}{t'(s)}\right) t', \\ &=: \int_{s_1}^{s_2} ds\, L_{ext}(t, q, t', q'), \end{aligned} \tag{3.18}$$

where a primed quantity refers to a derivative with respect to s. On the extended phase space, the Legendre transformations are defined by

$$\begin{aligned} p_t &= \frac{\partial}{\partial t'} L_{ext} = L\left(t, q, \frac{q'}{t'}\right) - \frac{q'}{t'} \frac{\partial}{\partial \frac{q}{t'}} L\left(t, q, \frac{q'}{t'}\right) \\ p_q &= \frac{\partial}{\partial q'} L_{ext} = \frac{\partial}{\partial \frac{q'}{t'}} L\left(t, q, \frac{q'}{t'}\right) \end{aligned} \tag{3.19}$$

Note that t' only appears in the quantity $\frac{q'}{t'}$ which is not dependent on the choice of parametrization. The Hamiltonian constraint is:

$$H = p_q q' + p_t t' - L_{ext} = t' C. \tag{3.20}$$

The Hamiltonian consists only of the constraint C (with t' as the Lagrange multiplier),

$$C = p_t + h, \tag{3.21}$$

where h is the Hamiltonian of the original theory

$$h = p_q \dot{q} - L(t, q, \dot{q}). \tag{3.22}$$

[3] The reparametrization of t by s needs to be monotonic.

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The key point here is that t' is an arbitrary function that does not affect the equations of motion on the constraint surface. The Hamiltonian H does not generate physical time evolution, but just pure gauge transformations[4], which reflects the freedom to change how t is reparametrized by s, which determines what the function $t' = \frac{dt}{ds}$ is.

The discussion above allows us to consider a few concepts. Firstly, a *partial observable* is defined as some real valued function of phase space whose values correspond to, in principle, physical measurement outcomes[5]. In the model that has just been discussed, one could imagine a clock that gave some time measurement, and a method of determining the position of the particle. The above correspond to t and q, respectively, which are in that sense partial observables.

Partial observables are not invariant under the gauge flow. In the current example, the gauge flow corresponds to the flow generated by the constraint C defined in equation (3.21). The the solutions to the equations of motion are $q(s)$ and $t(s)$. q and t evolve dynamically with s according to these solutions. A complete observable is one that is constructed from partial observables in a gauge invariant way. If one where to make an association between q and t, that is to specify $q(t)$, the value that q takes for any given value of t, then a 'complete' description of the system is attained, hence the term *complete observable* is used to describe the quantity $q(t)$. $q(t)$ in constructed in the following manner: if we seek the value that q takes when t takes the value τ, we would invert the solution to the equation of motion $t(s)$ for $s(t)$, to obtain the value of s for which $t = \tau$. Then, that value of s is plugged into the solution for $q(s)$, so that $q(t) = q(s(t))$. $q(t)$ can also be termed a '*relational observable*, in the sense that is a quantity that represents what the 'position' q is, when the 'clock' t reads a certain value (it relates physical quantities to each other). $q(t)$ is a gauge-invariant quantity for the system, because when one seeks the value of q when t takes on a particular value (say τ), the answer does not depend on the value of the parameter s. Everywhere along the orbit on which t changes with s, $q(t = \tau)$ is obtained by solving $t(s)$ for s in terms of t (to obtain the value of s for which $t = \tau$, and then inserting the result into the expression for q, in the manner $q(t) = q(s(t))$. The resulting value $q(t)$ is always the same, regardless of which parameter s is chosen.

We consider a simple example to make the above discussion more explicit. Consider the motion of a free, non-relativistic particle, with the mass set to $m = \frac{1}{2}$ for

[4]A system in which the dynamics is generated only by a constraint, rather than a true Hamiltonian, is termed *totally constrained*.

[5]An operational philosophy is not implied. The important thing is that partial observables assign numbers that have some 'physical' meaning.

convenience. The action is given by

$$S = \int dt \frac{\dot{q}^2}{4}\,, \tag{3.23}$$

where a $\dot{}$ denotes a derivative with respect to time, t. If the the particle is reparametrized by s and time promoted to a canonical variable with conjugate momentum p_t, the extended action, as defined in equation (3.18) for this system is

$$S_{ext} = \int ds \frac{(q')^2}{4t'}\,. \tag{3.24}$$

The momenta are

$$p_q = \frac{q'}{2t'}\,, \qquad p_t = -\frac{1}{4}\left(\frac{q'}{t'}\right)^2\,. \tag{3.25}$$

Immediately we recognize the constraint

$$C = p_q^2 + p_t\,, \tag{3.26}$$

and the Hamiltonian that generates the dynamics with respect to the parameter s is the constrained Hamiltonian

$$H = t'C\,. \tag{3.27}$$

t' acts as a Lagrange multiplier. If we choose $t' = 1$ which fixes the parametrization, then the equations of motion of the parametrized system are

$$\begin{aligned} t' &= \{t, C\} = 1 & p_t' &= \{p_t, C\} = 0 \\ q' &= \{q, C\} = 2p_q & p_q' &= \{p_q, C\} = 0\,. \end{aligned} \tag{3.28}$$

We immediately recognize p_t and p_q as Dirac observables. Additionally we have as solutions to the equations of motion:

$$t(s) = s + t \qquad q(s) = 2p_q s + q\,.$$

Now we can choose t as the 'clock', and denote the relational observables describing the evolution of q and p with respect to t as $Q(\tau)$ and $P(\tau)$. The relational observables are defined as the correlations of q and p with t, when t reads the value τ, that is

$$Q(\tau) = q(s)|_{t(s)=\tau}\,, \tag{3.29}$$

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and likewise for P. Having solved the equations of motion, we can write explicitly:

$$Q(\tau) = 2p_q(\tau - t) + q \qquad\qquad P(\tau) = p_q\,. \tag{3.30}$$

It is easy to show that $Q(\tau)$ commutes with the constraint, $\{Q(\tau), C\} = -2p_q + 2p_q = 0\ \forall\tau$, and hence is a Dirac observable as well. Thus we see explicitly, that the relational observable $Q(\tau)$ is gauge invariant. The two relational observables form a canonical pair $\{Q(\tau), P(\tau)\} = 1$. Hence $Q(\tau)$ and $P(\tau)$ describe gauge-invariant evolution of q and p with respect to t. This coincides with the original evolution in t (before reparametrization), because

$$\frac{\partial Q(\tau)}{\partial\tau} = 2p_q\,, \qquad\qquad \frac{\partial P(\tau)}{\partial\tau} = 0\,. \tag{3.31}$$

Indeed, this corresponds to equations of motion generated by the Hamiltonian $H = P^2(\tau) = p^2$, and the dynamics of the two relational observables is equivalent to the unconstrained dynamics defined by the original action, S in equation (3.23).

The extension as discussed above, will be an overkill for such a simple system. However, the ideas illustrated become important for gravitational systems which do not admit an absolute time. In gravitational systems, there is no unique time variable through which the dynamics of the theory can be described. 'Time evolution' is an idea that should be reconsidered conceptually, and that will be mainly to relate some physical quantities to others physical quantities (used as the 'clocks') as illustrated, that is, one extracts the dynamics by means of relational Dirac observables. This is a way in which physical dynamics can be extracted from a constrained Hamiltonian system.

We now make the above discussion more general. The complete or relational (Dirac) observable of interest, associated with a phase space function f and clock T, will be following construction, in the case of one constraint, C [27]:

$$F_{[f,T]}(\tau, x) := \alpha_C^t(f)(x)\big|_{\alpha_C^t(T)(x)=\tau}\,. \tag{3.32}$$

The notation requires some interpretation. T is the variable used as the 'clock'. f is a partial observable, that assigns a value $f(x)$ to each point on the constraint surface $\mathcal{C}$ corresponding to the value of some physical quantity. $\alpha_C^t(x)$ is the gauge orbit associated with the point x. The point reached on the gauge orbit from an initial point is parametrized by the real parameter t. Subsequently, $\alpha_C^t(f)(x)$ gives the value of the partial observable f evaluated at the point reached by moving along the gauge orbit for a 'time' t. The same applies for the clock, T.

In summary, $F_{[f,T]}(\tau, x)$ associates to the point x on the constraint surface the value $\alpha_C^{t_0}(f)(x)$, where the value of the parameter $t = t_0$ is given as that value of t that satisfies

$$\alpha_C^t(T)(x) = \tau. \tag{3.33}$$

This construction ensures that the complete observables are constant along the gauge orbit.

An important requirement is for the solution to (3.33) to be uniquely determined at every point on the constraint surface. The ability to satisfy this requirement is strongly dependent on the choice of the gauge parametrizing 'clock' variable T which is chosen. In general, $T(x)$ must be strictly monotonic along the gauge orbit[6].

The construction was generalized from flows generated by a single constraint, to gauge transformation generated by a constraint algebra by Dittrich [13]. Using the definition of a gauge transformation, one writes:

$$F_{[f,T^k]}(\tau^k, x) := \alpha_{\beta_i C_i}(f)(x)|_{\alpha_{\beta_i C_i}(T^k)(t)=\tau^k} \,. \tag{3.34}$$

The interpretation is the same, except that there is now a set of variables T^k with as many fixing parameters τ^k. The observable evaluates the phase space function f at the point on the gauge orbit reached by performing the gauge transformation that satisfies the condition

$$\alpha_{\beta_i C_i}(T^k)(x) = \tau^k. \tag{3.35}$$

It is required that this condition is met at a unique point on the gauge orbit. Thus, there should be as many independent gauge parametrizing clocks as there are independent constraints that generate the gauge orbit.

It can be shown that a formal expression for the complete observable is [14]

$$F_{[f,T^k]}(\tau^k) \approx \sum_{n=0}^{\infty} \frac{1}{n!}\{\cdots,\{\cdots,\{f,\tilde{C_{k_1}}\},\tilde{C_{k_2}}\}\cdots,\tilde{C_{k_n}}\}(\tau - T^{k_1})(\tau - T^{k_2})\cdots(\tau - T^{k_n}). \tag{3.36}$$

where $\tilde{C_k} := (A^{-1})^j_k C_j$. This expression is only a formal one, and obtaining an analytic solution in general is not necessarily easy. Additionally, one cannot a priori guarantee that the matrix A is invertible throughout phase space, or that the formal expression in terms of an infinite sum converges. In general, the properties of the observable are strongly dependent on the choice of T^k.

[6]Indeed, this was the reason why the parametrization in the example of the free particle was required to be monotonic.

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3.0.2 Reduced phase space and algebra of Dirac observables

Given a system with a Hamiltonian constraint, with trajectories that lie on the constrained surface $\mathcal{C}$, we can construct the space of solutions to the equations of motion. This is done by taking the quotient of the constraint surface by the gauge orbit. Specifically,

$$\mathcal{S} = \mathcal{C}/\sim, \tag{3.37}$$

where $\mathcal{S}$ is the space of solutions, and $\sim$ is the equivalence relation that identifies all points on a gauge orbit. For integrable systems, this usually defines a phase space, called the *reduced phase space* [16], but for chaotic systems, there will be no reduced phase space.

Functions defined over the reduced phase space are constant along the gauge orbits: these are precisely the Dirac observables. The reduced phase space inherits a Possion bracket structure, which is simply the Poisson bracket evaluated for the Dirac observables on the constraint hypersurfaces. Accordingly, Dirac observables form a Poisson algebra. Notice that since the Dirac observables commute with all the constraints, they are first class functions. As we have shown earlier in (2.26), first class functions form an algebra, since the Poisson bracket of two first class functions is also first class. Indeed, since the Hamiltonian constraint is itself a gauge-invariant quantity, dynamics in the reduced phase space, in terms of relations between the Dirac observables, is generated by an unconstrained Hamiltonian with a Poisson bracket structure. This was seen explicitly with the example of the reparametrized free particle. Recall that the Dirac observables defined there, $Q(\tau)$ and $P(\tau)$ admit the Poisson bracket structure $\{Q(\tau), P(\tau)\} = 1$ and relational dynamics generated by the Hamiltonian $H = P(\tau)^2$. Further details on the structure of the reduced phase space can be obtained in the text by Henneaux and Teitelboim [16].

A maximal set of independent Dirac observables is required to parametrize the reduced phase space. In order to obtain these observables, one needs to have a complete set of solutions to the equations of motion, as we have done with the example of the free particle. The existence of the reduced phase space which admits the Poisson bracket structure of the Dirac observables is dependent on the quotient space being a smooth manifold [16]. We will see in Section 5 of the thesis that aside the technical difficulties one may have in obtain a complete set of solutions to the equations of motion, the full set of Dirac observables required to obtain an algebra on the reduced phase space may not exist. Additionally, the existence of the Poisson bracket structure requires that the quotient space is a

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smooth manifold. We will show in Section 5 for a model that the quotient space is not a smooth manifold, and the reduced phase space with a Poisson algebra of Dirac observables does not exist.

So far, we have looked at constraints arising in the Hamiltonian formulation of theories with gauge (non-physical) degrees of freedom, and how one could suitably encode the physically relevant information of the theory. Dirac observables have been introduced, and Rovelli's scheme of complete observables has been discussed as an example of Dirac observables. The goal of this research thesis is to investigate the role that chaos in constrained Hamiltonian systems could potentially play in constructing Dirac observables. We shall see in a simple model that a reduced phase space and algebra of Dirac observables does not exist in the presence of chaos. In order to prepare for this, the following section reviews concepts regarding chaos in unconstrained Hamiltonian systems.

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Chapter 4

Chaos and non-integrability in unconstrained Hamiltonian systems

To understand the role chaos might play in gauge systems, we briefly discuss how chaos arises in unconstrained Hamiltonian systems. Chaotic dynamical systems are characterized by exponential separation of trajectories with neighbouring initial values[1]. This definition holds for motion that remains in some bounded region. Systems with chaotic motion are distinct from systems with regular motion, in which trajectories that start near to each other are only separated linearly for all time, as we shall see shortly.

This distinction is important, as there are dynamical systems in which motion of trajectories is apparently random only as a consequence of imprecision in the specification of the initial values. These systems may in fact be integrable systems with regular motion, and if their initial values were to be known with arbitrary precision, the motion can be integrated and arbitrarily close trajectories experience similar fates for all time. An example of such a system is the ideal roulette wheel.

If a system is indeed chaotic, it is an inherent property of the system's dynamics, and not a result of the knowledge (or lack thereof) of the initial values of trajectories. The precise mathematical definitions and characterization of chaotic systems differ in literature and in different contexts. Here, we consider how chaotic motion can arise in Hamiltonian systems: that is, systems described by the path a trajectory follows in phase space that conserves the Hamiltonian (or "energy") function of phase space variables, (q, p). Hamiltonian systems are a special class

[1] There are systems in which trajectories do not exponentially diverge, but will be described as chaotic in another sense. This will be discussed later in the section.

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of dynamical systems, particularly because by Liouville's theorem, Hamiltonian systems preserve phase space volume. More precisely, if a connected set of points in phase space it taken as initial values, and the system is allowed to evolve for a time, the image of the set of points under this flow is also a connected set in phase space, and has the same volume as the initial set. This property gives Hamiltonian systems nicer behaviour than other dynamical systems, and for instance excludes the occurrence of attractors. This is an important point to note, as attractors are frequently a cause for non-integrable behaviour in other classes of dynamical systems.

4.0.1 Integrable systems

Consider an autonomous Hamiltonian system (its Hamiltonian function is time independent). One says it is integrable if one can solve for the time-evolution of phase space variables to obtain analytic expressions. The techniques for solving the equations of motion differ depending on the system of interest, but the end result is the same: through elimination and integration, one can write down closed-form expressions for the phase space trajectories. Integrable systems can be more precisely defined and characterized using the following theorem (This theorem is outlined by Arnold [2]).

Theorem 4.0.1. *Suppose that there are N functions $F_1, \cdots F_N$ on a $2N$-dimensional symplectic manifold, M i.e. the phase space of a dynamical system with the Hamiltonian $H(q,p)$ and N degrees of freedom. Suppose also that the N functions on phase space satisfy*

$$\{F_i, F_j\} = 0 \tag{4.1}$$

for every pair i, j. In particular, let $H(q,p)$ be one of these N functions, such that equation (4.1) implies that all the functions are constants of motion with respect to the dynamics generated by the Hamiltonian H. The vector fields (see equations (3.2) and (3.3)) associated to the N functions $F_1, \cdots F_N$ generate a family of N-dimensional submanifolds M_F of M, where a given M_F is defined by specific values of $F_1, \cdots F_N$ (This is due to Frobenius' theorem). Then if

1. *the differentials of all the functions are linearly independent at each point of M_F*
2. *the vector fields are complete on M_F* [2]

[2]This means that the flow generated by the vector fields of each of the functions to which the vector fields are tangent exist always, or otherwise, the vector field nowhere vanishes on M_F.

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then

a) each connected component of M_F is diffeomorphic to $\mathbb{T}^k \times \mathbb{R}^{n-k}$ and

b) on $\mathbb{T}^k \times \mathbb{R}^{n-k}$ there exist coordinates $\theta_1, \cdots \theta_k$ mod 2π, $y_1, \cdots, y_{n-k}$ in which Hamilton's equations take the form:

$$\begin{aligned} \dot{\theta}_i &= \omega_i\,, \\ \dot{y}_j &= c_j\,, \end{aligned} \tag{4.2}$$

where the ω's and c's are constants, and the index i runs from 1 to k and the index j runs from 1 to $n-k$.

In this case the Hamiltonian system is said to be completely integrable.

Integrable systems are characterized by the existence of N constants of motion for N degrees of freedom. A few very simple examples are enumerated here:

1. Trivially, the motion of a free particle with a single degree of freedom is an integrable system. The Hamiltonian is the only required constant of motion for the system to be integrable, since phase space is 2-dimensional. The trajectory is a straight line in phase space given by $p = constant$ (which is not independent of the Hamiltonian). In this case, $M_F \simeq \mathbb{R}$.

2. The elliptic motion of a particle in a plane with an inverse square central force is a completely integrable system. The constants of motion are the energy ($H = \frac{p_1^2+p_2^2}{2m} + \frac{k}{q_1^2+q_2^2}$) and the angular momentum $L_z = q_1p_2 - q_2p_1$. Here two constants of motion are needed, since phase space is 4-dimensional for motion in a plane with 2 degrees of freedom. In this case, the trajectory in phase space is confined to a torus. Here, $M_f \simeq \mathbb{T}^2$.

3. One could combine the systems in the above examples into a composite system. Consider the elliptic motion of the particle in the plane, and then add a further degree of freedom by extending the motion to 3-dimensions, so that the particle moves in a plane which is translated along its perpendicular at a fixed rate. One would then have a 6-dimensional phase space, an additional term $\frac{p_3^2}{2m}$ to the Hamiltonian in the previous example, and one additional constant of motion, which is $p_3 = constant$. Trajectories in phase space will lie in a submanifold diffeormorphic to a $\mathbb{T}^2 \times \mathbb{R}$. This last example is included to cover all the cases distinguished by values that k in the statement of the theorem can take (namely $k = 0$, $0 < k < n$ and $k = n$).

Equations (4.2) highlight why neighbouring trajectories in integrable systems always have liner separation. For a given Hamiltonian, motion is constrained to surfaces diffeormorphic to $\mathbb{T}^k \times \mathbb{R}^{n-k}$. If two points, x_0 and x_0' near to each other on the surfaces of motion are taken as initial data, it is easy to see from the equations of motion that they are always linearly separated, since c and ω are constants.

In the theory of completely integrable Hamiltonian systems, the case where M_F is compact ($k = n$) is only a special case, and has been treated extensively because it is mathematically tractable (see for instance, Arnold et al [2]). In the compact case, there exist special symplectic coordinates I_i and θ_i mod 2π in which the Hamiltonian takes the form $H = H(I_i)$ and the equations of motion are $\dot{I}_i = 0$ and $\dot{\theta}_i = \omega(I_i)$. These coordinates are the so-called *action-angle variables*. The I's are the "actions": they label the invariant tori on which trajectories move for fixed energies. The θ's are the "angles", and they locate points on each torus. The name "angle" is appropriate, since the angle variables change by 2π after a complete circuit in each independent direction on the torus, for each of the angle variables (see Arnold [2] for details).

There is extensive work in understanding the compact case. In particular, there is the KAM theory (to be discussed soon) which covers one way in which chaos can arise, namely as a perturbation on an integrable system. However, the present discussion seeks to understand the consequences of chaos in gravitational systems. In the most general case, chaos need not arise from perturbations at all, let alone as a perturbation around invariant tori. Nevertheless, some understanding of the role of chaos may be gained by investigating specific scenarios.

4.0.2 Non-integrable systems

Non-integrable systems are those in which there exist no global constants of motion apart from the Hamiltonian which generates motion. Such systems may give rise to chaotic motion. Two classes of non-integrable systems, which are interesting for gravity are discussed here (see Berry [7], Ott [24] and Zaslavsky [34] for more details and other classes).

Ergodic Systems

In ergodic systems, almost all orbits eventually explore almost all points in a $(2N - 1)$-dimensional surface in phase space (the surface of constant energy $E = H$). Integrable systems as above are, in fact, a very special class of Hamiltonian

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systems. A generic Hamiltonian system has ergodic behaviour. Ergodicity may be associated with chaotic motion, but is not always necessarily the case. In particular, the $N = 1$ case is degenerate: it is trivially ergodic, since motion confined to a 1-dimensional surface necessarily fills all of the surface after long enough times; and it is integrable as well. For $N > 1$, ergodic systems may be chaotic.

One way of identifying chaos is to partition phase space into discrete cells of fixed volume, and study the order in which the cells are explored by trajectories: chaotic motion would generate random sequences, and two trajectories that were close together within an initial cell will traverse cells of very different sequences (Berry [7]).[3]

Quasi-integrable systems

Quasi-integrable systems are systems which have a Hamiltonian of the form:

$$H(q,p) = H_0(q,p) + \epsilon H_1(q,p). \tag{4.3}$$

H_0 is an integrable Hamiltonian, H_1 is a non-integrable Hamiltonian, and ϵ is a small parameter that turns on the non-integrable part as a perturbation. When $\epsilon = 0$, trajectories lie on invariant tori, if according to Theorem 4.1m M_F is compact. Subsequently, one would like to investigate what happens when the perturbation is turned on.

Systems of this type are particularly interesting as they, for instance, describe what happens in the solar system. If the mutual gravitational interactions between planets are ignored, each planet moves in elliptic Kepler orbits (that is, using Newton's theory of gravity as an inverse-square central force). The ignored gravitational effects can be accounted for by turning on a perturbative term of the type ϵH_1 (Arnold et al [2]). It turns out that quasi-integrable systems are neither integrable nor ergodic in the sense that neither property holds throughout all of phase space.

The answer to what the fate of an integrable system is under perturbation is provided by the Kolmogorov-Arnold-Moser (KAM) theory (see Arnold [2], Berry [7]). A very detailed exposition will fall outside the scope of this thesis. The main results will be shortly outlined.

Briefly, the theory states that for sufficiently small ϵ, most of the invariant tori of

[3]Ways of characterizing chaos in dynamical systems are discussed in slightly more detail a little later.

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the unperturbed Hamiltonian survive the perturbation.

To discuss what the statement that 'most of the tori survive' means more precisely, recall that if a system is integrable and M_F is compact, then one can perform a coordinate change into action-angle coordinates (I, θ) referred to earlier. The equations of motion (4.2) $\dot{\theta}_i = \omega_i$ mean that each of the angles processes at a constant rate ω_i. This describes how trajectories move on the tori. For each torus, the frequencies $\vec{\omega}$ are constant ($\vec{\omega}$ can be considered a vector of frequencies). Depending on what the frequencies are, there are two types of motion, outlined in the following definition:

Definition 4.0.1. *A torus $\mathbb{T}^N$ in phase space is said to be quasi-periodic, or non-resonant, if there is no vector of integers $\vec{m} \in \mathbb{Z}^N$ such that*

$$\vec{m} \cdot \vec{\omega} = 0.$$

Otherwise, the torus is periodic, or resonant.

On a resonant torus, the frequencies are pairwise rationally dependent (i.e. $\omega_i/\omega_j \in \mathbb{Q}, \forall i, j$). Consequently, after a finite time, a trajectory returns to the same point on the torus. On the other hand, a trajectory on a quasi-periodic torus has irrationally related frequencies and fills the surface of the torus densely as $t \to \infty$ [2]. The set of resonant tori (of the unperturbed Hamiltonian) is everywhere dense in phase space, but has zero Lebesgue measure.

One says that a torus of the unperturbed Hamiltonian survives the perturbation if there exists a torus in the perturbed ($\epsilon \neq 0$) phase space whose toroidal surface and orbit frequencies continuously approach those of the unperturbed torus as $\epsilon \to 0$. Only non-resonant tori survive perturbation, possibly in a deformed way. There is a precise condition which the unperturbed non-resonant tori must satisfy to guarantee their survival of the perturbation (the precise statement is relevant to one of the approaches to proving the theorem, which will not be detailed here, see Ott [24]). The statement that most of the tori survive the perturbation is a reflection of the fact that there is a 'very large' set of tori of the unperturbed Hamiltonian which satisfy this property and survive the perturbation.

The resonant tori (those for which there is some $\vec{m}$ such that $\vec{m} \cdot \vec{\omega} = 0$) do not survive the perturbation. Under a perturbation ($\epsilon \neq 0$), the region of phase space originally occupied by the resonant tori develop complicated dynamics, and there exist orbits with chaotic motion that fill regions of dimension $2N - 1$, because only H is constant, whereas before perturbation, they lived on invariant tori of dimension N.

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Compact integrable systems and the KAM theory provide and interesting case in which to understand the occurrence of chaos in Hamiltonian systems through perturbations, but the framework is very limiting for the current considerations. In the following we make a slightly more formal elaboration of what chaotic dynamics is, and discuss some quantifiers of chaos in dynamical systems in general.

4.0.3 Chaos: characterization and measures

The trouble with dealing with chaos is that the phenomenon of chaos is not uniquely defined mathematically. Which dynamical systems are considered chaotic depends on what one's precise definition of chaos is. It is important to point out here that a non-integrable or even an ergodic system is not necessarily chaotic, with respect to any of the standard definitions. Also, the different definitions of chaos which one could come up with are not necessarily compatible. Additionally, given some precise definition of chaos, and some means of determining whether a dynamical system is chaotic or not, it may generally be difficult to carry out the computation which is required to characterize the system as chaotic or not.

In order to make a meaningful discussion of the role chaos will play in systems of our interest, a more precise means of characterizing a given dynamical system as chaotic is needed. At the beginning of this section, two intuitive ideas about the dynamics of a system were referred to as being indicative of a system being chaotic. The first is, trajectories that are initially 'near' to each other exponentially separate as the system evolves. The second is the idea that chaotic motion introduces a quality of randomness in the behaviour of the system.

Exponential separation of trajectories can be quantified using so-called Lyapunov exponents. Also, the amount of randomness can be quantified using any of a number of entropies that measure the time rate of 'information growth' of the solution space of dynamical systems. The two ideas are described briefly below, and based on them, a characterization of chaos is given for the purposes of this thesis.

Lyapunov exponents

There exists a mathematically rigorous characterization of the quality of exponential divergence in terms of so-called Lyapunov exponents.

Lyapunov exponents are however problematic for general relativistic systems, because the idea of exponential divergence depends on the choice of time. This

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is admissible in the Newtonian case, but problematic for general relativity. Entropies, which are discussed below, are more suitable because they are constructed to characterize invariant properties of the entire solution space. Entropies are thus more useful to the current discourse, and Lyapunov exponents are not discussed further. A detailed discussion on Lyapunov exponents is carried out by Ott [24] and Zaslavsky [34].

Entropy of dynamical systems

An entropy is a measure of the complexity or information growth associated with the trajectories of a dynamical system. To understand how this works, suppose points in phase space can only be determined to a certain precision, ϵ. If two initial points are within a distance ϵ of each other, they would be indistinguishable. If the system is chaotic, the trajectories of the initial data might separate exponentially[4]. This separation makes the two initial points more distinguishable in time. Namely, if one follows a trajectory of the dynamical system, the further one goes into the future, the more precisely one can determine the origin of the trajectory in the past, with the given accuracy ϵ, despite having only had a resolution of accuracy ϵ to distinguish initial data. In this way, the dynamics of a chaotic system causes an increase in information. An entropy is generally zero for a system without chaos, and non-zero for a chaotic system.

Two entropy measures are introduced here, the *Kolmogorov-Sinai* (or *metric*) entropy [20, 29, 30], and the *topological* entropy [1]. In the following discussion, we consider entropy measures on a discrete system. The dynamics of the system are specified by a discrete time evolution map M, that takes a point in the solution space to another point in the solution space. In the case of continuous time Hamiltonian systems, this map can be derived from the Hamiltonian in such a way that it sequentially maps points on the trajectory to subsequent points on the trajectory in discrete time intervals.

The Kolmogorov-Sinai entropy is based on Shannon's entropy formulation [28], which measures the degree of uncertainty with which the outcome of a probabilistic event can be predicted. Consider an experiment with r different possible outcomes

[4]Or, at least, that trajectories which initially cannot be distinguished within ϵ precision experience very different fates in the solution space.

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with probabilities $p_1, p_2, \cdots, p_r$. The Shannon entropy is the quantity[5]:

$$H_S = \sum_{i=1}^{r} p_i \ln\left(\frac{1}{p_i}\right). \tag{4.4}$$

($p_i \ln(1/p_i) \equiv 0$ is defined for when $p_i = 0$). In one extreme case, if one of the outcomes is certain, say $p_1 = 1$ ($p_2 = p_3 = \cdots = p_r = 0$), then one obtains $H_S = 0$. There is no uncertainty in predicting the outcome of the experiment. In the other extreme case, all the outcomes are equally likely to occur ($p_1 = p_2 = \cdots = p_r$). The Shannon entropy in this case is maximal and reads $H_S = \ln r$. Thus $0 \leq H_S \leq \ln r$. The closer the entropy is to 0, the higher the predictability of the outcome is. On the other hand, if the entropy nears $\ln r$, then the certainty with which the outcome can be predicted is low.

To define the metric entropy for a dynamical system, consider W to be some bounded region with some measure ρ which is invariant under a discrete time evolution map M. W is the space in which trajectories lie. ρ plays the role of the probability measure. The statement 'ρ is invariant under M' in the case of Hamiltonian mechanics for instance, means that if ρ is a measure defined over phase space volume, it is unaffected by the evolution of the system, since Hamiltonian mechanics preserves phase space volume.

Next, construct a partitioning $\{W_i\}$ of W, consisting of r disjoint components, so that $W = W_1 \cup W_2 \cup \cdots \cup W_r$. One can define an entropy function, in analogy to (4.4) of the partition by

$$H(\{W_i\}) = \sum_{i=1}^{r} -\rho(W_i) \ln[\rho(W_i)]. \tag{4.5}$$

Next, we repartition W into a system of partitions with smaller and smaller sizes using the evolution map in the following way. Using the map M, form the sets $M^{-1}(W_k)$ of the original partitioning, and then for each pair of integers $j, k = 1 \cdots r$, form r^2 intersections

$$W_j \cap M^{-1}(W_k). \tag{4.6}$$

Define $\{W_i^{(2)}\}$ to be the set of non-empty intersections formed this way. The next step, $\{W_i^{(3)}\}$ is obtained by collecting the non-empty intersections

$$W_j \cap M^{-1} W_k \cap M^{-2} W_l, \tag{4.7}$$

[5]The capital letter 'H' defines an entropy measure and is not to be confused with a Hamiltonian. Where a Hamiltonian is meant, it will be explicitly stated.

with $j, k, l = 1, \cdots, r$. Subsequently, the n-th partitioning is

$$W_{i_1} \cap M^{-1} W_{i_2} \cap \cdots \cap M^{-(n-1)}(W_{i_n}), \tag{4.8}$$

with $i_1, i_2, \cdots, i_n = 1, 2, \cdots, r$. Next define the quantity:

$$H_{ks}(\rho, \{W_i\}) = \lim_{n \to \infty} \frac{1}{n} H(\{W_i^{(n)}\}), \tag{4.9}$$

where H on the right hand side of the above equation is defined in equation (4.5). The *Kolmogorov-Sinai* entropy, or KS entropy, is given as the maximum of this quantity over all possible initial partitionings ($\{W_i\}$),

$$h_{ks} = \sup_{\{W_i\}} H_{ks}(\rho, \{W_i\}). \tag{4.10}$$

The *topological entropy* follows a similar construction. Having defined the partitioning $\{W_i^{(n)}\}$, let $N^{(n)}(\{W_i^{(n)}\})$ be the number of non-empty elements of the partitioning $\{W_i^{(n)}\}$, and define

$$H_T(M, \{W_i\} = \lim_{n \to \infty} \left[\frac{1}{n} \ln N^{(n)}(\{W_i\}) \right], \tag{4.11}$$

then the topological entropy of M is

$$h_T(M) = \sup_{\{W_i\}} H_T(M, \{W_i\}). \tag{4.12}$$

The topological and metric entropy are not equivalent. One has in general [24]

$$h_T \geq h_{ks}. \tag{4.13}$$

Entropies are in general difficult to compute explicitly, though in some cases numerical computations are possible.

Entropies have some important and useful invariance properties [24]. The topological entropy is invariant under a class of transformations of the time evolution map M. Specifically, a system with an evolution map M', which is obtained from M via a continuous, invertible, but not necessarily differentiable change of phase space variables, has the same entropy as M. M' is said to be topologically conjugate to M. The metric entropy is invariant under isomorphisms (one-to-one but not necessarily continuous change of variables). These invariant properties make entropies important. Particularly, they safeguard the results entropy of measures from changing due to arbitrary changes in variables. This property is important

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in the context of gravitational systems.

Having discussed Lyapunov exponents and entropies, a dynamical system is characterized by the following: if a given dynamical system (or specifically, a Hamiltonian system), satisfies one or both of the following statements:

a) The motion of the system is bounded in phase space, and there is at least one positive Lyapunov exponent, resulting in instability of initial data.

b) One (or both) of the topological or Kolmogorov-Sinai entropies is non-zero.

then the dynamics of the system will be said to be chaotic. Note, however, that there exist other definitions of chaos (see [24, 34]).

To summarize what has been discussed so far, the first part of the thesis in section 2 discusses how gauge degrees of freedom are manifested in Hamiltonian systems with constraints. In section 3, we looked at the conceptual and technical issue of determining what the physical degrees of freedom of a theory are, and discussed schemes to encode these degrees of freedom using gauge-invariant quantities and relational dynamics. Section 4 is a general review of the phenomenon of chaos in unconstrained Hamiltonians as a special class of dynamical systems. This concludes the review portions of this thesis. In the last part of the thesis, we shall look at chaos in constrained Hamiltonian systems and the conceptual and technical challenges it causes for relational dynamics and Dirac observables, and the interpretation of dynamics.

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Chapter 5

Chaos and non-integrability in constrained systems

Chaos and non-integrability are typical, inherent features of generic Hamiltonian dynamics [2, 7, 24, 34]. Integrable systems (those systems that satisfy Theorem 4.1) are a rather special class of Hamiltonian systems. In unconstrained systems, non-integrability makes systems analytically intractable and poses technical challenges, but does not necessarily present conceptual challenges which affect how one interprets the theory. Constants of motion are not needed to interpret and evaluate the dynamics of the theory, such that their absence (other than the Hamiltonian) does not cause conceptual trouble. One does not need to solve the dynamics to access the physical degrees of freedom.

In the case of systems with constraints, as has been discussed earlier, not all dynamical degrees of freedom represent physically relevant information. In some theories, such as QED, there is a true Hamiltonian, as well as constraints which generate gauge degrees of freedom. Such systems still possess the notion of time-evolution generated by the Hamiltonian, and the non-physical degrees of freedom are dealt with by appropriate gauge-fixing choices. In totally constrained systems however, like general relativity, the Hamiltonian only consists of a constraint, and there is no external notion of physical time evolution. Thus, we would like to define quantities that are invariant along the gauge orbits to characterize the distinct physical states of the system. That is, we need to solve the dynamics to access the physical degrees of freedom. Having sufficiently many (depending on the number of degrees of freedom) of these quantities allows one to characterize the space of solutions to the system: these constant functions are the observables which 'label' the physically distinct solutions of the system.

However, a non-integrable (and possibly chaotic) system means there exist no

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smooth, global constants of motion apart from the Hamiltonian. For the constrained Hamiltonian systems, the Dirac observables will be the constants of motion of the constraints. Thus for a chaotic system with a Hamiltonian constraint, there are no Dirac observables, other than the constraints. Their absence poses a challenge for canonical theories that attempt to encode physical information by constructing Dirac observables. This issue seems to haven been largely ignored in the literature on Dirac observables, especially in a gravitational context. To understand and illustrate this discussion further, we consider the following simple toy model. To the best of the author's knowledge, this seems to be the first non-integrable and ergodic Hamiltonian constrained system discussed in the literature, where one can make the absence of a sufficient amount of Dirac observables and a reduced phase space explicit. This constitutes the research part of this thesis.

5.0.1 Free particle on a torus

Consider first a free particle moving in a two-dimensional plane, $\mathbb{R}^2$, with position degrees of freedom labelled x and y. If the particle is constrained to move with a total energy E, then the dynamics of the system is generated by the totally constrained Hamiltonian:

$$C_H = \frac{1}{2}\left(p_x^2 + p_y^2\right) - E\,, \tag{5.1}$$

where p_x and p_y are the momenta conjugate to x and y respectively. The solutions to the equations of motion are:

$$\begin{aligned} x(t) &= p_x t + x(0)\,, \\ y(t) &= p_y t + y(0)\,. \end{aligned} \tag{5.2}$$

The motion is clearly integrable, and in order to characterize the solutions, one can specify two Dirac observables. One of them is p_x, which automatically fixes $p_y \approx \pm\sqrt{2E - p_x^2}$ (the weak equality is used here to emphasize that this is only true on the constraint surface). The other is the z-component of angular momentum, $L_z = xp_y - yp_x$, since C_H is rotation invariant. Additionally, one can solve the system and relate y and x as a relational observable in the manner (i.e x is the relational 'clock' variable alluded to in Section 3.1):

$$y(x) = \frac{p_y}{p_x}\Big(x - x(0)\Big) + y(0)\,. \tag{5.3}$$

Nothing spectacular happens here, as the motion is integrable, and we have two

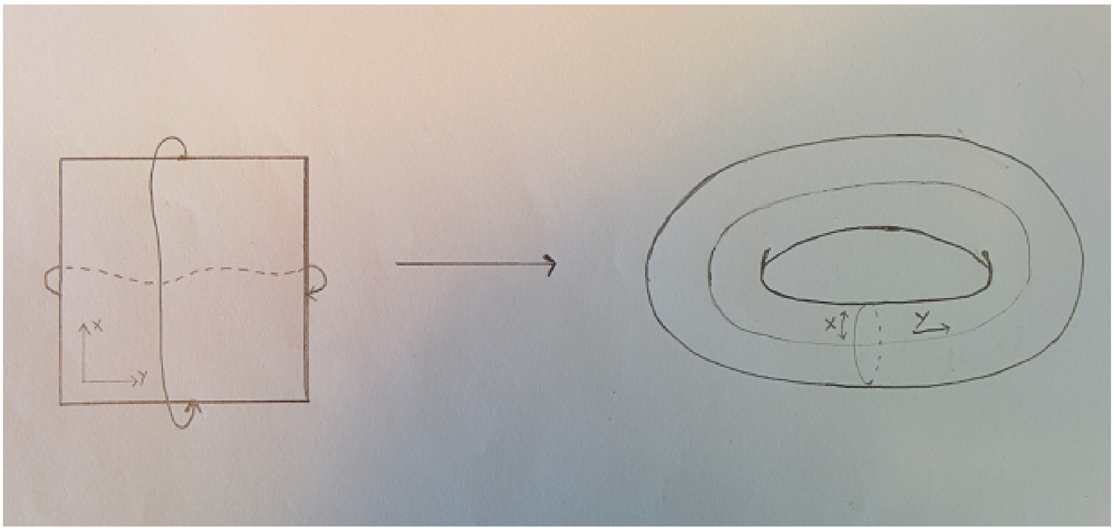

Figure 5.1: Motion in the two-dimensional plane is compactified to a torus. Here we identify the sides of a square of unit length in the plane. The curves drawn on the torus indicate how we label positions. On the longer curve, the x-coordinate is constant, and the y-coordinate varies. On the shorter curve, the y-coordinate is constant, and the x-coordinate varies.

observables. Now, we investigate what happens when the dynamics is compactified in the following way (see figure 5.1).

In the two-dimensional plane in which the particle moves, we make the identification:

$$\begin{aligned} x+1 &\sim x\,, \\ y+1 &\sim y\,. \end{aligned} \tag{5.4}$$

Then, the motion of the particle in position space is confined to a compact surface, namely a torus $\mathbb{T}^2$. Motion in four-dimensional phase space is restricted to the constraint surface:

$$\mathcal{C} \simeq I \times \mathbb{T}^2, \tag{5.5}$$

where I is the interval on $[-\sqrt{2E}, +\sqrt{2E}]$ to which p_x or p_y is restricted, and we have $x, y \in [0,1]$. The solutions to the equations of motion now take the form:

$$\begin{aligned} x(t) &= p_x t + x(0) - n(x,y) \\ y(t) &= p_y t + y(0) - m(x,y). \end{aligned} \tag{5.6}$$

$n(x,y)$ and $m(x,y)$ are called the 'winding numbers', which are piecewise constant functions that confine the position degrees of freedom to the torus. The winding numbers increase by 1 after each circuit in the x (n) and y (m) directions.

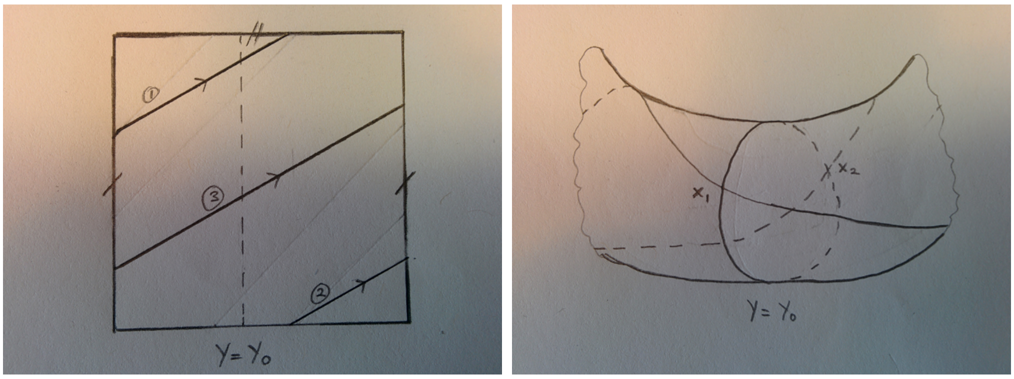

Figure 5.2: The diagram on the left shows a resonant trajectory with three branches superimposed on the unit square. Whenever a trajectory leaves the top border and reappears at the bottom border, the winding number $n(x, y)$ increases by one. If the trajectory leaves and reappears at the sides, the winding number $m(x, y)$ increases by one. If the initial point was a point on the line marked 1, and we indicate the branch of the solution by an ordered pair of winding numbers (n, m), the trajectory will follow the sequence of lines $1 \to 2 \to 3 \to 1$, and the branches will have the sequence $(0, 0) \to (1, 0) \to (1, 1) \to (1, 2) \to (2, 2) \to \cdots$. The diagram on the right shows a small portion of the torus. The closed loop corresponds to y fixed at y_0. When we seek the value of x when y takes the value y_0, there will be two solutions, shown by the two trajectories crossing the loop at x_1 and x_2. The situation is also marked on the figure on the left. If the torus is non-resonant, trajectories will not close in on themselves, and instead of a finite number of lines and crossings of the fixed y_0, there will be densely many, and illustrating the situation will essentially mean shading the pictures completely.

We could ask if Dirac observables as discussed in Section 3.1, on the constrained surface, can be found. p_x (which fixes, and is not independent of, p_y) applies as in the previous case. However, whether one can find another independent Dirac observable, such as L_z above, does not follow straightaway, as it was in the previous case. p_x parametrizes solutions in I. But for a fixed value of p_x, there is non-trivial dynamics on $\mathbb{T}^2$. p_x is constant for any of the trajectories on the torus, so we need another Dirac observable to parametrize the orbits on $\mathbb{T}^2$ for the fixed value of p_x.

Before the question of whether one can find another Dirac observable, independent of p_x, is answered, a certain consideration must be taken into account. Each value of p_x (which fixes p_y) within the allowed range of values gives rise to two possible cases:

1. There is first the case that p_x and p_y are rationally dependent, i.e. $\frac{p_x}{p_y} \in \mathbb{Q}$. In this case, the torus on which the particle moves is a resonant torus (as discussed in Section 4.2). On resonant tori, trajectories are closed and periodic.

2. The second case is when $\frac{p_x}{p_y} \notin \mathbb{Q}$. Here the torus is non-resonant according

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to Definition 4.1, and every trajectory fills the torus densely [2]. By dense filling, what is meant more precisely is that for every point $\tilde{x}_0(x, y)$ on the torus, every open neighbourhood $U_{\tilde{x}_0}$ of $\tilde{x}_0$ is intersected by every single one of the possible trajectories, for a fixed choice of p_x.

Now, the question of whether a second independent Dirac observable exists is addressed. Suppose that there exists such a quantity, $F(p_x, x, y)$, and that it is smooth. F need only depend on one of p_x or p_y explicitly, as one fixes the other. However, F must depend on either x, or y, or in other words, at least one of the statements $\frac{\partial F}{\partial x} \neq 0$ or $\frac{\partial F}{\partial y} \neq 0$ must be true. If this were not so, F would not be independent of p_x, which we require. For our system, we need two independent Dirac observables, and p_x is one of them: F would have to be the other, hence it must be independent of p_x. Then, the definition of a Dirac observable implies:

$$\{F, C_H\} = p_x \frac{\partial F}{\partial x} + p_y \frac{\partial F}{\partial y} \approx 0. \tag{5.7}$$

At this point, we can state a simple result as a theorem.

Theorem 5.0.1. *There does not exist a Dirac observable F, which is globally and continuously defined on $\mathcal{C}$, and satisfies equation (5.7) and is independent of p_x.*

Proof. By definition of F, it must take a constant value along every trajectory on $\mathcal{C}$. However, if the torus corresponding to some value of p_x is non-resonant, then trajectories densely fill the torus. Consequently, for any point on the torus, every open neighbourhood is intersected by every one of the trajectories on this torus. This, in turn, means that in every open neighbourhood of any point on the torus, F must take every one of its possible values on $\mathbb{T}^2$ for a fixed p_x. This implies F cannot be continuous.[1] This statement is true at every point on the torus. Thus, F is nowhere continuous; consequently, F is nowhere smooth on the torus. Hence, F fails to be smooth on $\mathcal{C}$. □

The conclusion of the above theorem is that one cannot define a Dirac observable on the constraint hypersurface apart from and independent of p_x or p_y. A Dirac observable must be a smooth function on the constraint hypersurface. The desire was to characterize the system by having enough (in this case, two) independent

[1]To make this conclusion clearer, note that for F to be continuous, then for F evaluated at some reference point $\tilde{x_0}(x, y)$ on $\mathbb{T}^2$, one needs to be able to make $|F(\tilde{x}) - F(\tilde{x_0})|$ arbitrarily small by choosing an arbitrarily small neighbourhood $|\tilde{x} - \tilde{x_0}|$ of $\tilde{x_0}$ (this, according to the neighbourhood definition of continuity). However, motion on a non-resonant torus is ergodic, so F takes all of its values in any open neighbourhood of any point on the torus, hence F fails to satisfy the condition of being continuous.

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Dirac observables O_i to parametrize the space of solutions to the system, as explained in section 3.2. Dirac observables would satisfy a Poisson algebra, $\mathcal{A}$, that is:

$$O_i, O_j \in \mathcal{A} \implies \{O_i, O_j\} \in \mathcal{A}. \tag{5.8}$$

Theorem 5.1 implies that we do not even have such an algebra of independent observables. This has severe repercussions: there can thus also not exist a reduced phase space (as discussed in Section 3.2). If there was a reduced phase space, the Poisson algebra of functions on it would imply an algebra of Dirac observables on $\mathcal{C}$ [16]. In the next section, we shall see that the reduced phase space is not even a manifold. Compactifying the free dynamics to a torus destroys the integrability of the system and the existence of smooth, global Dirac observables.

In the spirit of the relational observables discussed in section 3, we could consider the relation between y and x, and choose x as the relational clock variable for example, as was done earlier in equation (5.3). Then the relation can be written down using the solutions to the equations of motion (5.6) above. We would solve $x(t)$ for t and then insert into the expression for y, to obtain:

$$y(x, n, m) = \frac{p_y}{p_x}\Big(x - x_0 + n(x, y)\Big) + y_0 - m(x, y). \tag{5.9}$$

This expression is well-defined, albeit implicitly, because n and m depend on x and y. The meaning of the relation between the evolving y and x as a clock is a well-defined notion. In general, $y(x)$ will be multivalued. How many solutions exist for y as a function of x? Diagrammatically, for the resonant case, if some value of the clock x is fixed at a certain value, a trajectory crosses that x-coordinate a number of times. In other words, y will be multivalued for each reading of the clock variable x. This number, N_y corresponds to the number of complete revolutions in y, before the trajectory closes in on itself. This number is finite, since the motion is closed. An analogous argument holds in the opposite case, in which case y is chosen as the clock and x the evolving degree of freedom. Then, we would have N_x complete revolutions in x. On the other hand, in the non-resonant case, the problem has infinitely many solutions, as trajectories cross the loop fixed by the x-coordinate densely (See figure **??**). In summary:

1. In the resonant case, there exist N_y solutions for $y(x)$.
2. In the non-resonant case, there exist infinitely, but countably many solutions for $y(x)$. Hence, it is impossible to solve explicitly and globally for y as a function of x.

Although equation (5.9) cannot be solved globally, there do exist local solutions for

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both the resonant and non-resonant case. Specifically, solutions to the relational dynamics exist within every branch of the solutions to the equations of motion. A branch of the solutions to the equation of motion is defined by an admissible pair of winding numbers n and m. Within this branch, $y(x)$ is uniquely defined, and is simply a linear function.

5.0.2 Solution space of the free particle on a torus

In this section, we explicitly construct the space of solutions $\mathcal{S}$ to the equations of motion and investigate its properties. The constraint surface on which trajectories lie $\mathcal{C} \simeq I \times \mathbb{T}^2$ is a topological manifold. Each trajectory, τ_{p_x}, on $\mathcal{C}$, is characterized by a choice of p_x and initial data on $\mathbb{T}^2$. The solution space is constructed in the following manner.

The flow lines define an equivalence relation $\sim$ on $\mathcal{C}$

$$x \sim x' \leftrightarrow \alpha_C^t(x) = x' \,, \tag{5.10}$$

for some $t \in \mathbb{R}$ and $x, x' \in \mathcal{C}$. The solution space $\mathcal{S}$ is the quotient space

$$S = \mathcal{C}/\sim \;. \tag{5.11}$$

$\mathcal{S}$ is well-defined mathematically, but is it a manifold? One can define the quotient map Q as follows:

$$Q : \mathcal{C} \to \mathcal{S} \,, \tag{5.12}$$

$$x \to [x] \,,$$

where $[x]$ is the equivalence class of x defined by the relation $\sim$. That is, $[x]$ is the trajectory through x. Q maps every point on the constraint surface to its corresponding point in the solution space. Before proceeding, the following observation will be needed: according to the definition of open sets in quotient spaces, an open set U of $\mathcal{S}$ is a set whose pre-image, U' under the quotient map Q is open in $\mathcal{C}$. Hence $U' \subset \mathcal{C}$, U' open in $\mathcal{C}$ implies $U = Q(U')$ open in $\mathcal{S}$. We shall make use of this definition to show that $\mathcal{S}$ fails to be a manifold with two statements:

1. *$\mathcal{S}$ is not Hausdorff*. On a Hausdorff space $\mathcal{S}$, for any two distinct points s_1

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and s_2, there exist open neighbourhoods $U_{s_1} \subset \mathcal{S}$ of s_1 and $U_{s_2} \subset \mathcal{S}$ of s_2 such that

$$U_{s_1} \cap U_{s_2} = \emptyset\,. \tag{5.13}$$

We claim that one cannot do this for every pair of points in $\mathcal{S} = \mathcal{C}/\sim$. Let us label by τ_{p_x} a trajectory in the torus labelled by p_x. Let p_x give rise to a non-resonant torus. Since every τ_{p_x} fills this torus densely, every open set in $\mathcal{C}$ which is intersected by τ_{p_x} is also intersected by every other τ'_{p_x} with the same p_x. That is, all open sets in $\mathcal{S}$ containing τ_{p_x} (every trajectory τp_x corresponds to a point in $\mathcal{S}$) will also contain every other τ'_{p_x}, such that τ_{p_x} and τ'_{p_x} cannot be distinguished by non-intersecting neighbourhoods as in (5.13).

2. More significantly, $\mathcal{S}$ *is not a topological manifold*[2]. Suppose $\mathcal{S} = \mathcal{C}/\sim$ were a topological manifold. Then for all open sets U in $\mathcal{S}$, there exists a homeomorphism $f_U : U \to \mathbb{R}^n$, $n > 1$.[3] Then, again, by the definition of open sets in $\mathcal{S}$, U open in $\mathcal{S}$ implies that the pre-image U' of U under the quotient map Q $(U = Q(U'))$ is open in $\mathcal{C}$. Define the map $f_U \circ Q : U' \to \mathbb{R}^n$, and note that since Q is continuous, we must have [33]:

$$f_U \text{ is continuous } \iff f_U \circ Q \text{ is continuous }. \tag{5.14}$$

Such a composition should exist for any open set U' in $\mathcal{C}$.

Notice that $f_U \circ Q$ would be constant on trajectories in U'. However, we have shown before (See Theorem 5.1) that there exist neighbourhoods $U' \subset \mathcal{C}$ (intersecting non-resonant tori) such that no continuous map from U' to open neighbourhoods in $\mathbb{R}^n$, $n > 1$ exists[4] which is constant along all trajectories in U'. But then, by (5.14), for $U = Q(U')$ no homeomorphism $f_U : U \to \mathbb{R}^n$, $n > 1$, exists. Hence, $\mathcal{S}$ is not a manifold.

[2]A topological space $\mathcal{M}$ is a topological manifold if every open neighbourhood U in $\mathcal{M}$ is homeomorhpic to an open set in $\mathbb{R}^n$. Additionally, a homeomorphism between two topological spaces, X and Y, is a continuous map $f : X \to Y$ whose inverse f^{-1} exists and is continuous.

[3]$\mathcal{S}$ should be at least two-dimensional. Phase space is four-dimensional, the Hamiltonian constraint gives a three-dimensional constraint surface on which trajectories lie. Moding out the flow should give a two-dimensional manifold, if $\mathcal{S}$ was a manifold. Hence the mapping to $\mathbb{R}^n$, $n > 1$.

[4]It would require at least two independent continuous functions $U' \to \mathbb{R}$ constant along trajectories in U'.

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Chapter 6

Conclusion

We conclude this thesis with a brief review of the topics discussed. A discussion of the implications of the research results to the larger picture of gravitational systems and the quest for its quantum theory follows, and we end with a few issues that need further study, beyond what the thesis has covered.

The body of the thesis consists of two main parts. In the first part, section 2,3 and 4 give a review of well-known literature. In the second part, section 5 discusses the main research results of the project.

In section 2, we discussed theories with gauge degrees of freedom, and how constraints arise in such theories. We saw that first class constraints generate gauge transformations, and that the physically relevant information for a state was represented not just as a point, but as a continuum of points on the constraint surface, the gauge orbit.

In section 3, we discussed how one can extract the physically relevant information in the theory. Dirac observables were introduced as gauge-invariant quantities which would achieve this goal, and we saw a construction of relational (complete) observables as Dirac observables, with a simple example to illustrate the concepts. Section 3 concluded with a discussion on the reduced phase space, which admits a Poisson algebra of Dirac observables.

The main objective of this research thesis was to investigate the role that chaos and non-integrability may play in constrained Hamiltonian systems. Section 4 reviewed some concepts regarding chaos in unconstrained Hamiltonian systems, including integrability and non-integrability of unconstrained Hamiltonian systems, ergodicity, and discussed quantitative characterizations of chaos in dynamical systems.

Having concluded the review part of the thesis in the previous three sections, we

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addressed the goal of the project in section 5, which is the research part of the thesis. There, we discussed a toy model derived out of the uninteresting dynamics of a free particle in the two-dimensional plane. We showed for the toy model that its construction through a compactification of the dynamics in the plane to a torus broke down integrability. We saw as a consequence that portions of the space of trajectories featured ergodic orbits, and we showed that this feature made constructing a maximal set of Dirac observables needed to characterize the system impossible. Lastly, we constructed the space of solutions explicitly, and showed that it was not a manifold, and hence did not admit a Poisson algebra of Dirac observables.

What is the significance of this toy model and the results obtained from it? Indeed, the model is simple, and not physically interesting. However, it allowed us to explicitly illustrate qualitative features we expect to be true of real gravitational systems. Chaos and non-integrability are generic features of dynamical systems. Nonetheless, while chaos and the potential technical challenges it poses for gravitational systems have been discussed in the literature [13, 17, 31], to the best of the author's knowledge, this is the first model in the literature that explicitly reveals these features.

As outlined in the introduction, there is strong evidence that general relativity constitutes a chaotic or at least a non-integrable system. This poses potential challenges for building a quantum theory.

Chaos in constrained systems is not extensively treated in the literature. A few exceptions are noted. Hoehn et al [17] discuss the non-integrability of the above mentioned FRW cosmological model and the absence of a global clock variable. They discuss how relational evolution can be realized locally, analogous to the situation seen with the toy model where one can solve the relational dynamics on each branch of the trajectories.

Chaos poses technical challenges to the program of relational dynamics and Dirac observables. In section 4, we discussed chaos in unconstrained system, but we emphasize that there is no issue in that setting, because one does not need to solve the dynamics of the system completely to access the physical degrees of freedom. The situation is different in constrained Hamiltonian systems. There, one needs to solve the dynamics to construct relational Dirac observables, as we did for the example of the free particle in section 3. Unfortunately, non-integrability will make this impossible. The highlight of this thesis is in the research part in section five where we constructed a model to expose these issues. We showed that the solution space is not even a manifold, and there does not exist a maximal set of Dirac observables sufficient for a Poisson algebra on a reduced phase space.

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Why are these qualitative properties important? This discussion has consequences for building a quantum theory. The existence of a Poisson algebra is often assumed for constrained systems. However, where this algebra is absent, and the reduced phase space manifold on which the physical information is encoded cannot be constructed, there exists no Poisson algebra to promote to a commutator algebra in the quantum theory. That is, the reduced phase space quantization is impossible in this case. These problems are however not fatal for the meaning of relational dynamics. As we have seen with the toy model, local notions of relational dynamics exist, but cannot be extended globally.

Now we could ask the question on what could be done to address these technical issues. A few points are considered. In one instance, it is possible to carry out Dirac quantization, which does not require a reduced phase space. One would quantize the full theory the usual canonical way, and then solve the constraints. There is the possibility that this circumvents the problem of trying to construct observables in the classical theory. But there, one has the challenge of understanding the relationship between the observables that one realizes in the quantum theory, and the observables of the classical theory.

One school of thought argues that we should not treat Hamiltonian constraints as generators of gauge symmetries, thus we should in principle not be computing Dirac observables as quantities that commute with the constraints in the first place [21]. For instance, Barbour et al [4] argue that Dirac's argument for first class constraints as generators of gauge transformation is invalid in reparametrization invariant theories.

One last point we will mention here is that there exists theories that avoid the problem of a gravitational system appearing as a constrained Hamiltonian. One of such, the so-called "shape dynamics", constructs gravity as foliations of spatial hypersurfaces with a spatial conformal invariance [15]. The result of this approach is a theory that has a true Hamiltonian which generates dynamics. Another approach in this group is Horava's "quantum gravity at a Lifshitz point" [18].

In conclusion, we point out issues not covered in the body of this thesis for further considerations. One of them arises from the fact that for the breakdown of the reduced phase space to occur in the toy model, it was sufficient that the compactified dynamics was non-integrable and possessed ergodic behaviour in parts of the space of trajectories. One could in principle attempt to compute the entropy, in order to confirm the existence of chaos in the entropic sense.

Lastly, as earlier alluded to, it may be possible to avoid these issues in the quantum theory by performing a Dirac quantization. This quantization can indeed be

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carried out. It turns out that one finds that the quantum theory can be solved, but it excludes trajectories on non-resonant tori [1]. We would like to understand better the relationship between the picture obtained in the quantized theory, and the original phase space that included non-resonant tori because of which the reduced phase space manifold did not exist.

[1]Unpublished work at the date of this thesis, by Philipp Höhn Bianca Dittrich and Tim Koslowski

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