Chapter 1

Introduction

This chapter gives an overview of some of the topics that will be covered so the reader can get a coherent picture of the types of problems and associated mathematical structures that will be developed.[1]

1.1 The Classical Water Molecule and the Ozone Molecule

An example that will be used to illustrate various concepts throughout these lectures is the *classical (non-quantum) rotating "water molecule"*. This system consists of three particles interacting by interparticle conservative forces (one can think of springs connecting the particles, for example) so that the total energy of the system, which will be taken as our Hamiltonian, is the sum of the kinetic and potenial energies. This system is shown in Figure 1.1.1. The interesting special case of three equal masses gives the "ozone" molecule.

We use the term "water molecule" mainly for terminological convenience. The full problem is of course the classical ***three body problem*** in space. However, thinking of it as a rotating system evokes certain constructions that we wish to illustrate.

Imagine this mechanical system rotating in space and, simultaneously, undergoing vibratory, or *internal* motions. We can ask a number of questions:

- How does one set up the *equations of motion* for this system?

[1] We are grateful to Oliver O'Reilly, Rick Wicklin, and Brett Zombro for providing a helpful draft of the notes for an early version of this lecture.

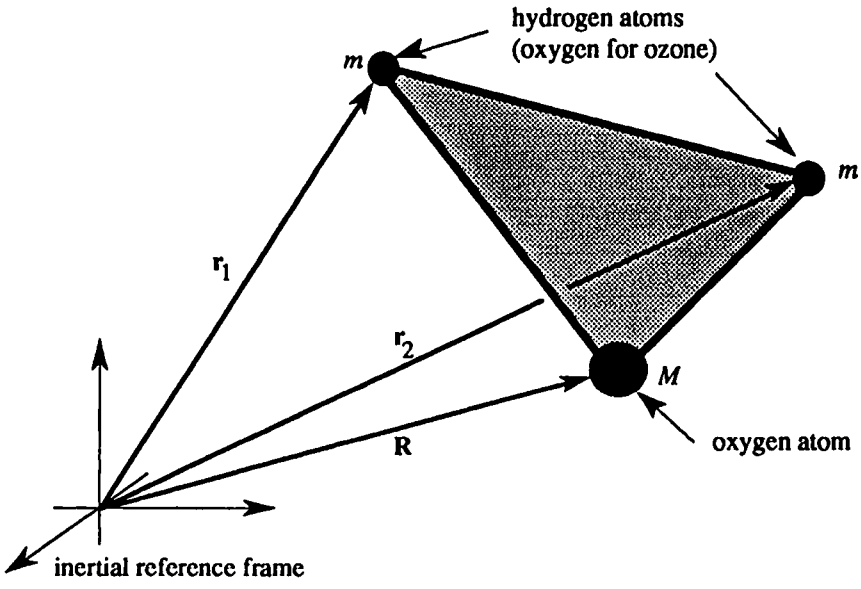

Figure 1.1.1: The rotating and vibrating water molecule.

- Is there a convenient way to describe *steady rotations*? Which of these is stable? When do bifurcations occur?
- Is there a way to separate the *rotational* from the *internal motions*?
- How do vibrations affect overall rotations? Can one use them to *control* overall rotations? To *stabilize* otherwise unstable motions?
- Can one separate symmetric (the two hydrogen atoms moving as mirror images) and non-symmetric vibrations using a discrete symmetry?
- Does a deeper understanding of the classical mechanics of the water molecule help with the corresponding quantum problem?

It is interesting that despite the old age of classical mechanics, new and deep insights are coming to light by combining the rich heritage of knowledge already well founded by masters like Newton, Euler, Lagrange, Jacobi, Laplace, Riemann and Poincaré, with the newer techniques of geometry and qualitative analysis of people like Arnold and Smale. I hope that already the classical water molecule and related systems will convey some of the spirit of modern research in geometric mechanics.

The water molecule is in fact too hard an example to carry out in as much detail as one would like, although it illustrates some of the general theory quite nicely. A simpler example for which one can get more detailed information (about relative equilibria and their bifurcations, for example) is the ***double spherical pendulum***. Here, instead of the symmetry group being the full (non-abelian) rotation group $SO(3)$, it is the (abelian) group S^1 of rotations about the axis of gravity. The double pendulum will also be used as a thread through the lectures. The results for this example are drawn from Marsden and Scheurle [1992]. To make similar progress with the water molecule, one would have to deal with the already complex issue of finding a reasonable model for the interatomic potential. There is a large literature on this going back to Darling and Dennison [1940] and Sorbie and Murrell [1975]. For some of the recent work that might be important for the present approach, and for more references, see Xiao and Kellman [1989] and Li, Xiao and Kellman [1990].

The special case of the ozone molecule with its three equal masses is also of great interest, not only for environmental reasons, but because this molecule has more symmetry than the water molecule. In fact, what we learn about the water molecule can be used to study the ozone molecule by putting $m = M$. A big change that has very interesting consequences is the fact that the discrete symmetry group is enlarged from "reflections" $\mathbb{Z}_2$ to the "symmetry group of a triangle" D_3. This situation is also of interest in chemistry for things like molecular control by using laser beams to control the potential in which the molecule finds itself. Some believe that, together with ideas from semiclassical quantum mechanics, the study of this system as a classical system provides useful information. We refer to Pierce, Dahleh, and Rabitz [1988], Tannor [1989] and Tannor and Jin [1991] for more information and literature leads.

1.2 Hamiltonian Formulation

The equations of motion for a classical mechanical system with n degrees of freedom may be written as a set of first order equations in Hamiltonian form:

$$\dot{q}^i = \frac{\partial H}{\partial p_i}; \quad \dot{p}^i = -\frac{\partial H}{\partial q_i}; \quad i = 1, \ldots, n. \tag{1.2.1}$$

The configuration coordinates $(q^1, \ldots, q^n)$ and momenta $(p_1, \ldots, p_n)$ together define the system's instantaneous state, which may also be regarded as the coordinates of a point in $\mathbb{R}^{2n}$, the system's ***phase space***. We denote such a point by (q, p). The Hamiltonian function $H(q, p)$ defines the system and, in the absence of constraining forces and time dependence, is simply

the total energy of the system. The phase space for the water molecule is $\mathbb{R}^{18}$ and the Hamiltonian is the kinetic plus potential energies.

This classical setting can be generalized in two essential ways. First, the phase space may be a higher dimensional surface (*i.e.*, a differentiable manifold) rather than a linear vector space. This generalization allows for the simplest and most natural characterizations of systems consisting of bodies whose motions are spatially constrained and for a deeper understanding even of an n-particle system like the water molecule. The set of all possible spatial positions of bodies in the system is their ***configuration space***. For example, the configuration space for the water molecule is $\mathbb{R}^9$ and for a three dimensional rigid body moving freely in space is $SE(3)$, the six dimensional group of Euclidean (rigid) transformations of three-space, that is, all possible rotations and translations. If translations are ignored and only rotations are considered, then the configuration space is $SO(3)$. As another example, if two rigid bodies are connected at a point by an idealized ball-in-socket joint, then to specify the position of the bodies, we must specify a single translation (since the bodies are coupled) but we need to specify two rotations (since the two bodies are free to rotate in any manner). The configuration space is therefore $SE(3) \times SO(3)$. This is already a fairly complicated object, but remember that one must keep track of both positions and momenta of each component body to formulate the system's dynamics completely. If Q denotes the configuration space (only positions), then the corresponding phase space P (positions and momenta) is the manifold known as the ***cotangent bundle*** of Q, which is denoted by T^*Q. This is a good way to generalize the phase space of an n-degree of freedom system.

The second important way in which the modern theory of Hamiltonian systems generalizes the classical theory is by relaxing the requirement of using canonical phase space coordinate systems, *i.e.*, coordinate systems in which the equations of motion have the form (1.2.1) above. Rigid body dynamics, celestial mechanics, fluid and plasma dynamics, nonlinear elastodynamics and robotics provide a rich supply of examples of systems for which canonical coordinates can be unwieldy and awkward. The free motion of a rigid body in space is a basic example of this type. It was treated by Euler in the eighteenth century and yet it remains remarkably rich as an illustrative example. Notice that if our water molecule has *stiff* springs between the atoms, then it behaves nearly like a rigid body. One of our aims is to bring out this behavior.

As mentioned earlier, the rigid body problem in its primitive formulation has the six dimensional configuration space $SE(3)$. This means that the phase space, $T^*SE(3)$ is twelve dimensional. Assuming that no external forces act on the body, conservation of linear momentum allows us to solve

for the components of the position and momentum vectors of the center of mass. Reduction to the center of mass frame, which we will work out in detail for the classical water molecule, reduces one to the case where the center of mass is fixed, so only $SO(3)$ remains. Each possible orientation corresponds to an element of the rotation group $SO(3)$ which we may therefore view as a configuration space for all non-trivial motions of the body. Euler formulated a description of the body's orientation in space in terms of three angles between axes that are either fixed in space or are attached to symmetry planes of the body's motion. The three *Euler angles*, ψ, φ and θ are generalized coordinates for the problem and form a coordinate chart for $SO(3)$. However, it is simpler and more convenient to proceed more intrinsically as follows.

We regard the element $A \in SO(3)$ giving the configuration of the body as a map of a ***reference configuration*** $\mathcal{B} \subset \mathbb{R}^3$ to the current configuration $A(\mathcal{B})$ taking a reference or label point $X \in \mathcal{B}$ to a current point $x = A(X) \in A(\mathcal{B})$. For a rigid body in motion, the matrix A becomes time dependent and the velocity of a point of the body is $\dot{x} = \dot{A}X = \dot{A}A^{-1}x$. Since A is an orthogonal matrix, we can write

$$\dot{x} = \dot{A}A^{-1}x = \omega \times x,$$

which defines the ***spatial angular velocity.*** The corresponding ***body angular velocity*** is defined by

$$\Omega = A^{-1}\omega,$$

so that Ω is the angular velocity as seen in a body fixed frame. The kinetic energy is the usual expression

$$K = \frac{1}{2}\int_{\mathcal{B}} \rho(X)\|\dot{A}X\|^2 d^3X,$$

where ρ is the mass density. Since

$$\|\dot{A}X\| = \|\omega \times x\| = \|A^{-1}(\omega \times x)\| = \|\Omega \times X\|,$$

the kinetic energy is a quadratic function of Ω. Writing

$$K = \frac{1}{2}\Omega^T \mathbb{I}\Omega$$

then defines the ***moment of inertia tensor*** $\mathbb{I}$, which we can regard as a positive definite 3×3 matrix, or better, quadratic form. This quadratic

form, can be diagonalized, and this defines the ***principal axes and moments of inertia.*** In this basis, we write $\mathbb{I} = \text{diag}(I_1, I_2, I_3)$. Every calculus text teaches one how to compute moments of inertia! The ***body angular momentum*** is defined, analogous to linear momentum $p = mv$, as

$$\Pi = \mathbb{I}\Omega$$

so that in principal axes,

$$\Pi = (\Pi_1, \Pi_2, \Pi_3) = (I_1\Omega_1, I_2\Omega_2, I_3\Omega_3).$$

The equations of motion for the rigid body are the Euler-Lagrange equations for the Lagrangian L equal to the kinetic energy, but regarded as a function on $TSO(3)$ or equivalently, Hamilton's equations with the Hamiltonian equal to the kinetic energy, but regarded as a function on the cotangent bundle of $SO(3)$. In terms of the Euler angles and their conjugate momenta, these are the canonical Hamilton equations, but as such they are a rather complicated set of six ordinary differential equations.

Assuming that no external moments act on the body, the spatial angular momentum vector $\pi = A\Pi$ is conserved in time. As we shall recall in Chapter 2, this follows by general considerations of symmetry. Euler used this to write the three associated momentum equations for the components of the body angular momentum vector obtaining the ***Euler equations***:

$$\begin{aligned} \dot{\Pi}_1 &= \frac{I_2 - I_3}{I_2 I_3}\Pi_2\Pi_3 \\ \dot{\Pi}_2 &= \frac{I_3 - I_1}{I_3 I_1}\Pi_3\Pi_1 \\ \dot{\Pi}_3 &= \frac{I_1 - I_2}{I_1 I_2}\Pi_1\Pi_2 \end{aligned} \tag{1.2.2}$$

Around 1966, it was Arnold who clarified in a satisfactory way the relationships between the various representations (body, space, Euler angles) of the equations and showed how the same ideas apply to fluid mechanics as well; see Arnold [1966].

Viewing (Π_1, Π_2, Π_3) as coordinates in a three dimensional vector space, the Euler equations are evolution equations for a point in this space. An integral (constant of motion) for the system is given by the magnitude of the total angular momentum vector: $\|\Pi\|^2 = \Pi_1^2 + \Pi_1^2 + \Pi_1^2$. This can be verified directly from the Euler equations (1.2.2). Because of this, the evolution in time of any initial point $\Pi(0)$ is constrained to the sphere $\|\Pi\|^2 = \|\Pi(0)\|^2 = \text{constant}$. Thus we may view the Euler equations as describing a two dimensional evolution on an invariant sphere. This sphere

is the ***reduced phase space*** for the rigid body equations. In fact, this defines a two dimensional system as a Hamiltonian dynamical system on the two-sphere S^2. The Hamiltonian structure is not obvious from Euler's equations because the description in terms of the body angular momentum is inherently non-canonical. As we shall see in §1.3 and in more detail in Chapter 4, the theory of Hamiltonian systems may be generalized to include Euler's formulation. The Hamiltonian for the reduced system is

$$H = \frac{1}{2}\left(\frac{\Pi_1^2}{I_1} + \frac{\Pi_2^2}{I_2} + \frac{\Pi_3^2}{I_3}\right) \tag{1.2.3}$$

and we shall show how this function allows us to recover Euler's equations (1.2.2). Since solutions curves of (1.2.2) are confined to the level sets of H (which are in general ellipsoids) as well as to the invariant spheres $\|\Pi\| =$ constant, the intersection of these surfaces are precisely the trajectories of the rigid body, as shown in Figure 1.2.1.

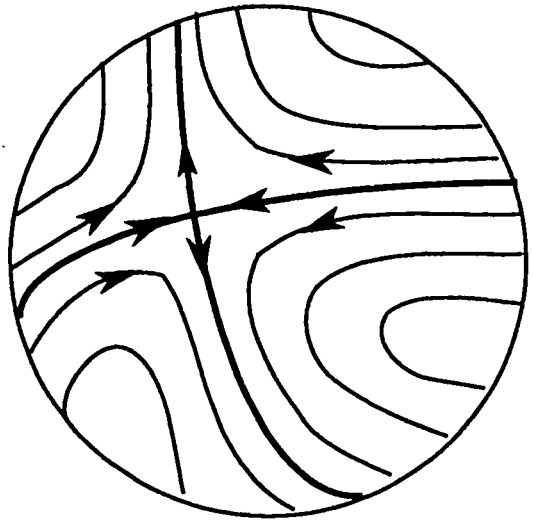

Figure 1.2.1: Phase portrait for the rigid body. The magnitude of the angular momentum vector determines a sphere. The intersection of the sphere with the ellipsoids of constant Hamiltonian gives the trajectories of the rigid body.

On the reduced phase space dynamical fixed points are called ***relative equilibria***. These equilibria correspond to periodic orbits in the unreduced

phase space, specifically to *steady rotations* about a principal inertial axis. The locations and stability types of the relative equilibria for the rigid body are clear from Figure 1.2.1. The four points located at the intersections of the invariant sphere with the Π_1 and Π_2 axes correspond to pure rotational motions of the body about its major and minor principal axes. These motions are stable, whereas the other two relative equilibria corresponding to rotations about the intermediate principal axis are unstable.

In these lectures we shall see how the stability analysis for a large class of more complicated systems can be simplified through a careful choice of non-canonical coordinates. We managed to visualize the trajectories of the rigid body without doing any calculations, but this occurrence is rare; the rigid body is an especially simple system. Problems like the rotating water molecule will prove to be more challenging. Not only is the rigid body problem integrable (one can write down the solution in terms of integrals), but the problem reduces in some sense to a two dimensional manifold and allows questions about trajectories to be phrased in terms of level sets of integrals. Many Hamiltonian systems are not integrable and trajectories are chaotic and are often studied numerically. The fact that we were able to reduce the number of dimensions in the problem (from twelve to two) and the fact that this reduction was accomplished by appealing to non-canonical coordinates turns out to be a general feature for Hamiltonian systems with symmetry. The reduction procedure may be applied to non-integrable or chaotic systems, just as well as to integrable ones. In a Hamiltonian context, non-integrability is generally taken to mean that any analytic constant of motion is a function of the Hamiltonian. We will not attempt to formulate a general definition of chaos, but rather use the term in a loose way to refer to systems whose motion is so complicated that long-term prediction of dynamics is impossible. It can sometimes be very difficult to establish whether a given system is chaotic or non-integrable. Sometimes theoretical tools such as "Melnikov's method" (see Guckenheimer and Holmes [1983] and Wiggins [1988]) are available. Other times, one resorts to numerics or direct observation. For instance, numerical integration suggests that irregular natural satellites such as Saturn's moon, Hyperion, tumble in their orbits in a highly irregular manner (see Wisdom, Peale and Mignard [1984]). The equations of motion for an irregular body in the presence of a non-uniform gravitational field are similar to the Euler equations except that there is a configuration-dependent gravitational moment term in the equations that may render the system non-integrable.

The evidence that Hyperion tumbles chaotically in space leads to difficulties in numerically modelling this system. The manifold $SO(3)$ cannot be covered by a single three dimensional coordinate chart such as the Euler angle chart. We shall prove this in §1.6. Hence an integration algorithm

using canonical variables must employ more than one coordinate system, alternating between coordinates on the basis of the body's current configuration. For a body that tumbles in a complicated fashion, the body's configuration might switch from one chart of $SO(3)$ to another in a short time interval, and the computational cost for such a procedure could be prohibitive for long time integrations. This situation is worse still for bodies with internal degrees of freedom like our water molecule, robots, and large-scale space structures. Such examples point out the need to go beyond canonical formulations.

1.3 Geometry, Symmetry, and Reduction

We have emphasized the distinction between canonical and non-canonical coordinates by contrasting Hamilton's (canonical) equations with Euler's equations. We may view this distinction from a different perspective by introducing Poisson bracket notation. Given two smooth (C^∞) real-valued functions F and K defined on the phase space of a Hamiltonian system, define the ***canonical Poisson bracket*** of F and K by

$$\{F, K\} = \sum_{i=1}^{n} \left(\frac{\partial F}{\partial q^i} \frac{\partial K}{\partial p_i} - \frac{\partial K}{\partial q^i} \frac{\partial F}{\partial p_i} \right) \tag{1.3.1}$$

where (q^i, p_i) are conjugate pairs of canonical coordinates. If H is the Hamiltonian function for the system, then the formula for the Poisson bracket is the directional derivative of F along the flow of Hamilton's equations; that is,

$$\dot{F} = \{F, H\}. \tag{1.3.2}$$

In particular, Hamilton's equations are recovered if we let F be each of the canonical coordinates in turn:

$$\dot{q}^i = \{q^i, H\} = \frac{\partial H}{\partial p_i}, \quad \dot{p}_i = \{p_i, H\} = -\frac{\partial H}{\partial q^i}.$$

Once H is specified, the chain rule shows that the statement "$\dot{F} = \{F, H\}$ for all smooth functions F" is equivalent to Hamilton's equations. In fact, it tells how any function F evolves along the flow.

This representation of the canonical equations of motion suggests a generalization of the bracket notation to cover non-canonical formulations. As an example, consider Euler's equations (1.2.2). Define the following non-canonical ***rigid body bracket*** of two smooth functions F and K on the angular momentum space:

$$\{F, K\} = -\Pi \cdot (\nabla F \times \nabla K), \tag{1.3.3}$$

where $\{F, K\}$ and the gradients are evaluated at $\Pi = (\Pi_1, \Pi_2, \Pi_3)$. The notation in (1.3.3) is that standard scalar triple product operation in $\mathbb{R}^3$. If H is the rigid body Hamiltonian (see (1.2.3)) and F is, in turn, allowed to be each of the three coordinate functions Π_i, then the formula $\dot{F} = \{F, H\}$ yields the three Euler equations.

The non-canonical bracket corresponding to the reduced free rigid body problem is an example of what is known as a ***Lie-Poisson*** bracket. Other bracket operations have been developed to handle a wide variety of Hamiltonian problems in non-canonical form, including some problems outside of the framework of traditional Newtonian mechanics (see for instance, Arnold [1966] or Marsden et al., [1983]). In Hamiltonian dynamics, it is essential to distinguish features of the dynamics that depend on the Hamiltonian function from those that depend only on properties of the phase space. The generalized bracket operation is a geometric invariant in the sense that it depends only on the structure of the phase space. The phase spaces arising in mechanics often have an additional geometric structure closely related to the Poisson bracket. Specifically, they may be equipped with a special differential two-form called the ***symplectic form***. The symplectic form defines the geometry of a symplectic manifold much as the metric tensor defines the geometry of a Riemannian manifold. Bracket operations can be defined entirely in terms of the symplectic form without reference to a particular coordinate system.

The classical concept of a canonical transformation can also be given a more geometric definition within this framework. A canonical transformation is classically defined as a transformation of phase space that takes one canonical coordinate system to another. The modern analogue of this concept is a ***symplectic map***, a smooth map of a symplectic manifold to itself that preserves the symplectic form or, equivalently, the Poisson bracket operation.

The geometry of symplectic manifolds is an essential ingredient in the formulation of the reduction procedure for Hamiltonian systems with symmetry. We now outline some important ingredients of this procedure and will go into this in more detail in Chapters 2 and 3. In Euler's problem of the free rotation of a rigid body in space (assuming that we have already exploited conservation of linear momentum), the six dimensional phase space is $T^*SO(3)$ — the cotangent bundle of the three dimensional rotation group. This phase space $T^*SO(3)$ is often parametrized by three Euler angles and their conjugate momenta. The reduction from six to two dimensions is a consequence of two essential features of the problem:

1. Rotational invariance of the Hamiltonian, and
2. The existence of a corresponding conserved quantity, μ, the *spatial*