Regularization and Quantization of the Kepler Problem

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Preface

This thesis contains the results of my master research in Mathematics at the Radboud University Nijmegen, which I did under the supervision of Prof. Gert Heckman. I looked at several mathematical structures that underly the Kepler problem, which models the motion of a particle in a $\frac{1}{q}$ potential. Eventually, I focussed on the theory that has to do with the regularization and quantization of the Kepler problem, and in particular on the relation with spherical and hyperbolic geometry, which I chose as the main topic of this text.

The aim is to describe and unify two regularizations of the classical Kepler problem by looking at the structure of the energy surfaces and the phase space, and to discuss the quantum analogue of one of them. Heuristically speaking, in this text the method of exhibiting the mathematical structure of the Kepler problem comes down to interchanging the position and momentum coordinates and to map the resulting system to a Riemannian manifold with constant curvature.

The text aims to point out the analogies between the bounded motions and the unbounded ones. I try to give a conceptual overview, and do not present all lengthy calculations. In the literature, often only bounded motions are considered. It is well-known that in this case many results have to do with spherical geometry. It is less known that analogous results are often true for the second case, but now in the setting of hyperbolic geometry. In this text, I aim to emphasize the similarity between the two cases. I will not prove every result twice, but I will briefly explain the similarities and the differences between them. Where possible, we consider the d-dimensional Kepler problem, rather than specifying the dimension. The physical motivation, however, comes from the three-dimensional Kepler problem, although other dimensions have turned out to be important in theoretical physics as well.

The first chapter contains a physical, i.e. mathematically non-rigorous, introduction to the Kepler problem, and is written as a motivation for the rest of this text. The following two chapters contain some mathematical preliminaries, namely symplectic geometry, which is necessary to understand the geometry of the classical Kepler problem; and the geometry of spheres and hyperboloids, which is needed for both the classical and the quantum Kepler problem. If the reader is acquainted with one or more of these subjects, he can skip the corresponding section(s).

After the mathematical preliminaries, the geometry of the classical Kepler problem is discussed. First, Kepler's laws are derived for the d-dimensional problem. Then we discuss and generalize the result by Moser, which relates Kepler orbits to geodesics. In particular, this method regularizes the energy surfaces. Subsequently, we discuss the Ligon-Schaaf regularization map, which regularizes the phase space of the Kepler problem at once, without distinguishing between the energy surfaces. At the end, we discuss the relation between the two regularizations.

Then the quantization of the Kepler Hamiltonian is discussed. The Hamilton op-

erator that arises naturally is not essentially self-adjoint, so there is no unique time-evolution of the quantum system. In fact, choosing a particular self-adjoint extension, is equivalent to fixing some unitary time-evolution. After giving some basic results about self-adjoint extensions, we discuss the possible self-adjoint extensions of the quantum Kepler Hamiltonian, distinguishing the dimensionality of the problem, and describe the choice usually made in the literature.

In the last part of this text, we discuss the quantum Kepler problem. First we treat the oldest derivation of the spectrum of the hydrogen atom by Pauli. He did this by looking at the hidden symmetries of the Kepler problem. We describe these in the language of Lie algebras and their representations. Then we discuss Fock's method, which is the quantum analogue of Moser's work. We also discuss at which point the choice of the self-adjoint extension of the quantum Kepler Hamiltonian is made. We end with pointing out the relation between Pauli's and Fock's approaches.

This text is not intended to prove new mathematical results. However, there are some additions to the literature, in particular connections between different approaches. For example, the explicit proof of the Moser regularization for positive energies has not been discussed in the literature so far. However, this result was suggested before and merely consists of transforming the spherical arguments to the hyperbolic setting. The relation between the Moser map and the Ligon-Schaaf map that is given in this text is new. However, I think that still more can be said about it. Finally, the discussion in which way Fock's method contains a choice of the self-adjoint extension of the Hamiltonian is an expected result, but I did not find this anywhere else.

I assume that the reader has at least the level of a master student in mathematics or mathematical physics. Therefore, I only give the more specific preliminaries as described above. Strictly speaking, no physics knowledge is needed. However, it is convenient to know something about classical and quantum mechanics.

I will consider d-dimensional spaces rather than spaces of a specific dimension. The set of natural numbers $\mathbb{N}$ is the set $\{1, 2, 3, 4, \dots\}$. I will write $\mathbb{N}_0$ for the set $\mathbb{N} \cup \{0\}$.

Manifolds are considered to be real and smooth. All Hilbert spaces are assumed to be complex, and all operators are linear and defined on a dense domain that is not necessarily the whole Hilbert space.

Vectors in and three-dimensional spaces are denoted in boldface. In this case, its length is denoted by q. In (arbitrary) d-dimensional spaces, the notation of vectors does not differ from the notation of scalars. The context should clarify if a quantity is a vector or a scalar. If it is convenient, we may denote a vector by its components. The length of a vector a is denoted by $\|a\|$.

Tim de Laat, Nijmegen, 11th August 2010

Contents

Chapter 1

The Kepler problem

The **classical Kepler problem** is to determine the trajectories of two particles interacting by a central force proportional to the inverse square of the distance between them. The **quantum Kepler problem** is to determine the wave functions of two particles interacting by such a force.[1] The explicit form of the force is given by:

$$\mathbf{F} = -\frac{k}{q^3}\mathbf{q}, \tag{1.1}$$

where k is some real constant, called the **coupling constant**. If $k > 0$, then the force is attractive. If $k < 0$, it is repulsive. In our treatment we assume that all quantities are dimensionless.

The Kepler problem has a very long history. The earliest and most motivating example of two bodies interacting with a force of the form of equation (1.1), is a planet moving around the sun, neglecting the interactions with other planets. There have been many attempts to describe the trajectories of planets, which we do not discuss. For our purposes, the modern treatment of the problem started at the end of the 16^{th} century. At his observatory, the astronomer Tycho Brahe (1546-1601) collected a large set of very accurate data of the positions of the planets in our solar system at different times. Johannes Kepler (1571-1630) used these data for his description of planetary motion, which culminated in his three laws:

1. the orbit of every planet is an ellipse with the sun at one of its foci (1605);
2. the line connecting the sun and a planet sweeps out equal areas in equal intervals of time (1602);
3. the square of the period of a planet is proportional to the cube of the semi-major axis of its orbit (1619).

[1] The difference between the definitions of both problems is remarkable. In the classical case, we look for time-dependent trajectories, but in the quantum case, we will eventually look for eigenfunctions of the time-independent Schrödinger equation.

It is an interesting fact that Kepler derived these laws using only Brahe's data, rather than any theoretical framework about mechanics, which had not yet been invented at that time.

In 1687, the brilliant Isaac Newton published his *Philosophiae Naturalis Principia Mathematica*, in which he lays the groundwork of classical mechanics. In this book, he states his three **laws of motion** and his **law of universal gravitation**.

The laws of motion are as follows:

1. in the absence of a force, a body is either at rest or moves along a straight line with constant velocity;

2. a body subdued to a force $\mathbf{F}$ experiences an acceleration $\mathbf{a}$ determined by the formula $\mathbf{F} = m\mathbf{a}$, where m is the mass of the body;

3. if a first body exerts a force $\mathbf{F}$ on a second one, then the second body exerts a force $-\mathbf{F}$ on the first one.

The law of universal gravitation says that all bodies attract each other. A mass m_A exerts a force $\mathbf{F_{AB}}$ on another mass m_B given by:

$$\mathbf{F_{AB}} = -G\frac{m_A m_B}{q_{AB}^3}\mathbf{q_{AB}},$$

where $\mathbf{q_{AB}}$ is the distance vector $\mathbf{q_B} - \mathbf{q_A}$ between m_A and m_B pointing towards m_B. G is a proportionality constant, called the universal constant of gravitation. Note that this force is of the form of equation (1.1).

One of the many important results in Newton's book is the derivation of Kepler's laws from Newton's laws, which was an extraordinary achievement at that time. Although he invented differential and integral calculus partly with the purpose of describing mechanical systems, in his book Newton obtained most results by means of geometric reasoning.

Another realization of the Kepler problem is given by two charged particles interacting by the Coulomb force, which is given by the following formula:

$$\mathbf{F_{AB}} = \frac{1}{4\pi\varepsilon_0}\frac{Q_A Q_B}{q_{AB}^3}\mathbf{q_{AB}}, \tag{1.2}$$

where Q_A and Q_B are the charges of the particles, $\mathbf{q_{AB}}$ is defined as above for the gravitational force and ε_0 is the electric constant. This force is either attractive (if the charges have different signs) or repulsive (if the charges have equal signs). In the first case, the force is essentially the same as the gravitational force.

The general form of the force in the Kepler problem is given by equation (1.1). By Newton's second law, a force implies an acceleration, because $\mathbf{F}$ equals $m\mathbf{a} = m\ddot{\mathbf{q}}$. Therefore, solving the Kepler problem means solving the following two differential

equations with specified initial conditions:

$$m_A \ddot{\mathbf{q}}_\mathbf{A} = -\frac{k}{q_{BA}^3}\mathbf{q_{BA}},$$
$$m_B \ddot{\mathbf{q}}_\mathbf{B} = -\frac{k}{q_{AB}^3}\mathbf{q_{AB}}.$$

If we define the **center of mass** z and the **reduced mass** μ as follows:

$$\mathbf{z} = \frac{m_A\mathbf{q_A} + m_B\mathbf{q_B}}{m_A + m_B},$$
$$\mu = \frac{m_A m_B}{m_A + m_B},$$

then the system decouples to the following system of differential equations:

$$\begin{aligned} \ddot{\mathbf{z}} &= 0, \\ \mu\ddot{\mathbf{q}} &= -\frac{k}{q^3}\mathbf{q}, \end{aligned} \tag{1.3}$$

where $\mathbf{q} = \mathbf{q_B} - \mathbf{q_A}$. Together, equations (1.3) are called the **reduced Kepler problem**. From the first equation we conclude that center of mass moves along a straight line with constant velocity. For solving the second equation it is convenient to use the Hamiltonian formalism. For a thorough introduction to this formalism, cf. [1, 2]. We only give a brief introduction to its underlying mathematical framework, symplectic geometry, in Chapter 2. An important advantage of Hamiltonian dynamics is that it depends largely on scalar-valued quantities, such as the **Hamiltonian** H, rather than on vector-valued ones. The value of H corresponds to the value of the energy. The Hamiltonian of the reduced Kepler problem is as follows:

$$H = \frac{p^2}{2\mu} - \frac{k}{q},$$

where $\mathbf{p}$ denotes the momentum of the particle. Physically, this Hamiltonian is the energy of a particle in a $\frac{1}{q}$ potential. It turns out that there are three essentially different types of trajectories that solve the second equation, corresponding to the situations $H < 0$, $H > 0$ and $H = 0$. We will briefly describe these situations now and will come back to these in Chapter 4.

- $H < 0$: In this case, $k > 0$. The particle follows an ellipse with the origin, which is the center of mass of the two particles, at one of the foci of the ellipse.

- $H > 0$: In this case, k can be positive as well as negative and hence the force can either be attractive or repulsive. The particle moves along a component of an hyperbola. If $k > 0$, then the trajectory is along the component closest to the center of mass. If $k < 0$, then the trajectory is along the other component.

- $H = 0$: In this case, $k \geq 0$. If $k = 0$, then the particle is free and hence moves along a straight line with constant velocity. If $k > 0$, the particle moves along a parabola with the origin at its focus.

It should be pointed out that for a given system we have a given value of k, which can be either positive, negative, or zero. The possible signs of the Hamiltonian follow from this, and we should distinguish these cases. However, we presented the possible forms of the trajectories by distuinguishing in the sign of H, because this determines the nature of the orbits. The case of planets orbiting the sun, as originally studied by Newton, corresponds to the case $H < 0$.

Another advantage of the Hamiltonian formalism is that the reduced Kepler problem can be generalized to d dimensions in a straightforward way. Two masses m_A and m_B interact by a central force $F(q) = F(\|q\|)\frac{q}{\|q\|}$, which is explicitly given by

$$F(q) = -\frac{k}{\|q\|^3}q$$

with $k \in \mathbb{R}$. Recall that our notation of a vector in d dimensions is different from the three-dimensional case.

After defining the center of mass z and the reduced mass μ in the same way as above, we obtain a decoupled system of equations given by:

$$\begin{aligned} \ddot{z} &= 0, \\ \mu\ddot{q} &= -\frac{k}{\|q\|^3}q, \end{aligned} \tag{1.4}$$

where $q = q_B - q_A$. This is the same system as given by equations (1.3), but with the three-dimensional vectors replaced by their d-dimensional analogues. Again, we conclude that the center of mass moves along a straight line with constant velocity. In the rest of this text, we are only concerned with the second equation of the set of equations (1.4). We will simply call this the **Kepler problem** rather than the d-dimensional reduced Kepler problem.

There are several methods, which even go back to Kepler and Newton, that give explicit methods of determining the trajectory of the particle. Obviously, to obtain a unique solution one needs to specify certain conditions, such as the initial values of position and momentum.

The force F is conservative, so it can be written as $-\nabla V$, where V is a (scalar) potential. Obviously, $V = -\frac{k}{\|q\|}$. Hence, the Hamiltonian H of the n-dimensional Kepler problem is given by:

$$H = \frac{\|p\|^2}{2\mu} - \frac{k}{\|q\|}. \tag{1.5}$$

So far, we only introduced the classical Kepler problem. It has a quantum analogue, in the sense that there are quantum systems that are described by the Schrödinger equation with a Kepler Hamiltonian. Physically, an example of such a quantum system

is the hydrogen atom. In this system, the particles interact by an attractive Coulomb force, as given in equation (1.2). This example even generalizes to scattering states, since this force may also be repulsive, namely in the case of charges with the same sign.

A more detailed approach to the quantum Kepler problem is given in this text at the time we need it. However, a more specific definition of the quantum Kepler problem is needed than was given at the beginning of this chapter. We say that the **quantum Kepler problem** consists of solving the Schrödinger equation for the quantum Kepler Hamiltonian. In this text, we will not give a complete solution to the quantum Kepler problem, since this is extensively done in the literature, and requires a lot of technicalities and lengthy calculations. We will, however, describe the quantum analogue of our classical treatment and say something about its geometry.

Chapter 2

Symplectic geometry

Symplectic geometry is the branch of differential geometry that deals with symplectic manifolds, i.e. manifolds equipped with a closed, non-degenerate, smooth two-form. Mathematicians were inspired to study such manifolds by the theory of Hamiltonian dynamics. Indeed, one of the motivating examples of a symplectic manifold is the cotangent bundle, which has a local chart given by the canonical coordinates q_i and p_i from mechanics.

We only state some basic facts and results about symplectic geometry. For a good introduction to the subject, cf. [6]. There one can also find the proofs we omit.

2.1 Symplectic manifolds

Definition 2.1.1. A **symplectic manifold** is a pair (M, ω) such that M is a C^∞ manifold with a closed, nondegenerate smooth two-form ω, called the **symplectic form**, defined on it, i.e. ω is a C^∞ map that assigns to every $p \in M$ a nondegenerate anti-symmetric bilinear form ω_p on T_pM and $d\omega = 0$.

The following proposition is a consequence of the nondegeneracy of a symplectic form.

Proposition 2.1.2. Symplectic manifolds are even-dimensional.

Remark 2.1.3. A symplectic manifold is called a symplectic vector space if the underlying manifold has the structure of a vector space. In this case, the symplectic form is just a nondegenerate, anti-symmetric bilinear form.

Example 2.1.4. A straightforward but very important example of a symplectic vector space, and hence also of a symplectic manifold, is $(\mathbb{R}^{2n}, \omega_0)$ with canonical base $e_1 = (1, 0, \ldots, 0), \ldots, e_n, f_1, \ldots, f_n = (0, \ldots, 0, 1)$, i.e.

$$\begin{aligned} \omega(e_i, e_j) &= \omega(f_i, f_j) = 0, \\ \omega(e_i, f_j) &= \delta_{ij}. \end{aligned}$$

We can explicitly write the symplectic form as:

$$\omega_0 = \sum_{i=1}^{n} e_i^* \wedge f_i^* =: \sum_{i=1}^{n} dx_i \wedge dy_i,$$

where e_i^* and f_i^* denote the dual vectors of e_i and f_i respectively.

Definition 2.1.5. A **symplectomorphism** is a diffeomorphism ϕ from a symplectic manifold (M, ω) to another symplectic manifold (M', ω') such that $\phi^*\omega' = \omega$, i.e. for all $p \in M$ we have $(\phi^*\omega')_p = \omega_p$, where $(\phi^*\omega')_p(u, v) = (\omega')_{\phi(p)}(d\phi_p(u), d\phi_p(v))$ for $u, v \in T_pM$.

Remark 2.1.6. Later in this text, we sometimes construct maps between symplectic manifolds that are not symplectomorphisms, but respect the symplectic structure in a weaker way. We describe this when we use it.

There is no global classification of symplectic manifolds. There is, however, a classification theorem for symplectic vector spaces and a local classification theorem for symplectic manifolds.

Theorem 2.1.7. Let (V, ω) be a symplectic vector space. Then (V, ω) is symplectomorphic to $(\mathbb{R}^{2n}, \omega_0)$ for some $n \in \mathbb{N}$.

Theorem 2.1.8 (Darboux-Weinstein)**.** Two symplectic manifolds are locally symplectomorphic if and only if they have the same dimension.

We will discuss an example of a symplectic manifold other than a symplectic vector space at the end of this chapter. It will turn out to be very important for the rest of this text.

2.2 Hamiltonian formalism

Let (M, ω) be a symplectic manifold of dimension $2n$. Recall Cartan's formula for the Lie derivative $\mathcal{L}$ of a smooth p-form α on a manifold M:

$$\mathcal{L}_X \alpha = \iota_X d\alpha + d(\iota_X \alpha), \tag{2.1}$$

where X is a vector field on M, ι is the interior product of X and α, and d is the exterior derivative.

Definition 2.2.1. A vector field X on M is called a **symplectic vector field** if $\mathcal{L}_X \omega = 0$.

Proposition 2.2.2. Let X be a vector field on a symplectic manifold (M, ω). Then the following are equivalent:

1. X is symplectic;

2. $\iota_X\omega$ is closed, i.e. $d(\iota_X\omega) = 0$;

3. $\iota_X\omega = df$ locally for some $f \in C^\infty(M)$, i.e. for all $x \in M$ there is an open set U with $x \in U$ and a smooth $f : M \to \mathbb{R}$ such that $\iota_X\omega = df$ in U.

Proof. Suppose X is symplectic. Then $0 = \mathcal{L}_X\omega = \iota_X d\omega + d(\iota_X\omega)$. Since ω is closed, we have $d(\iota_X\omega) = 0$.

Suppose $\iota_X\omega$ is closed. By Poincaré's Lemma[1], closed forms on smooth manifolds are locally exact, so there is an $f \in C^\infty(M)$ such that $\iota_X\omega = df$ locally.

It is sufficient to check the last implication in local charts. Let U be some chart. We have $\iota_X\omega = df$ in U. Then $\mathcal{L}_X\omega = \iota_X d\omega + d(\iota_X\omega) = 0$ in U, because ω is closed, $\iota_X\omega = df$ and $d^2 f = 0$. □

We have just considered vector fields X with some special property, namely that $\iota_X\omega$ is closed. We now consider what happens if they are exact. This is a stronger condition, since the third equivalence of the property then holds globally.

Proposition 2.2.3. If $H \in C^\infty(M)$, then there is a unique vector field X_H such that $\iota_{X_H}\omega = dH$.

Proof. Existence follows from the fact that at each point $x \in M$ there is a map from T_xM to T_x^*M given by $\xi \mapsto \omega(\xi, .)$ This is an isomorphism by nondegeneracy of ω. To each one-form dH we can assign the image X_H under the inverse isomorphism. Uniqueness also follows, because ω is nondegenerate. □

Definition 2.2.4. A vector field X such that $\iota_X\omega = dH$ for some $H \in C^\infty(M)$, i.e. $\iota_X\omega$ is exact, is called a **Hamiltonian vector field** and H the associated **Hamiltonian**. We denote by X_H the Hamiltonian vector field corresponding to the Hamiltonian H.

Remark 2.2.5. There is a linear map $C^\infty(M) \to \mathrm{Ham}(M)$, where $\mathrm{Ham}(M)$ denotes the set of Hamiltonian vector fields on M, given by $H \mapsto X_H$. This map is surjective by definition of $\mathrm{Ham}(M)$.

Proposition 2.2.6. If X and Y are symplectic vector fields on M, then $[X, Y]$ is a Hamiltonian vector field with Hamiltonian function $\omega(Y, X)$.

Proof. Using $\iota_{[X,Y]} = [\mathcal{L}_X, \iota_Y]$ and Cartan's formula, which is given in equation (2.1), we obtain:

$$\iota_{[X,Y]} = \iota_X d\iota_Y\omega + d\iota_X\iota_Y\omega - \iota_Y\iota_X d\omega - \iota_Y d\iota_X\omega = d(\omega(Y, X)).$$

This proves the claim. □

[1]Poincaré's Lemma says that on a contractible manifold, all closed forms are exact. Differentiable manifolds are locally contractible, so we can use this Lemma locally. For a proof of Poincaré's Lemma in the local case, cf. [1, Theorem 2.4.17].

Remark 2.2.7. The symplectic vector fields and the Hamiltonian vector fields form Lie-subalgebras of the Lie-algebra of vector fields.

Definition 2.2.8. For $f, g \in C^\infty(M)$, we define their **Poisson bracket** by $\{f, g\} := \omega(X_f, X_g)$.

Remark 2.2.9. It follows that

$$\{f, g\} = \omega(X_f, X_g) = \iota_{X_g}\iota_{X_f}\omega = \iota_{X_g} df = X_g(f) = \mathcal{L}_{X_g} f = -\mathcal{L}_{X_f} g.$$

Proposition 2.2.10. A function $f \in C^\infty(M)$ is constant along the integral curves of X_H for some $H \in C^\infty(M)$ if and only if

$$\{H, f\} = 0.$$

Proof. If ρ_t denotes the flow of X_H, then $(f \circ \rho_t)$ denotes the value of f along integral curves. We have:

$$\frac{d}{dt}(f \circ \rho_t) = \rho_t^* \mathcal{L}_{X_H} f = \rho_t^* \omega(X_f, X_H) = \rho_t^* \{f, H\},$$

where ρ_t^* denotes the pullback of the flow. From this, the result follows. □

Remark 2.2.11. A function f that is constant along integral curves of X_H is called an **integral of motion** with respect to H.

Proposition 2.2.12. Let X_H be a complete Hamiltonian vector field and let $\rho_t : M \to M$ for $t \in \mathbb{R}$ be its flow. Each diffeomorphism ρ_t is a symplectomorphism.

Proof.

$$\frac{d}{dt}\rho_t^* \omega = \rho_t^* \mathcal{L}_{X_H} \omega = \rho_t^* (d\iota_{X_H}\omega + \iota_{X_H} d\omega) = 0.$$

□

Remark 2.2.13. In this way, every smooth function on M produces a family of symplectomorphisms by the flow of its Hamiltonian vector field.

The next result follows from Proposition 2.2.6.

Proposition 2.2.14. $\{.,.\}$ is a Lie bracket. Moreover, it satisfies the Leibniz rule:

$$\{f, gh\} = \{f, g\}h + g\{f, h\},$$

for all $f, g, h \in C^\infty(M)$.

Proof. Bilinearity of $\{.,.\}$ follows from the bilinearity of ω and the linearity of the map $H \mapsto X_H$ described earlier. The other properties follow from elementary calculations. □

Definition 2.2.15. An **abstract Poisson bracket** on a commutative algebra A is a Lie bracket on A satisfying the Leibniz rule. A commutative algebra with a Poisson bracket defined on it is called a **Poisson algebra**.

If (M, ω) is a symplectic manifold, then $(C^\infty(M), \{.,.\})$ is a Poisson algebra. The following example gives an explicit formula for the Poisson bracket in canonical coordinates.

Example 2.2.16. On $(\mathbb{R}^{2n}, \omega_0)$, where $\omega_0 = \sum_{i=1}^n dx_i \wedge dy_i$, we have:

$$\iota_{\frac{\partial}{\partial y_i}}\omega = -dx_i,$$
$$\iota_{\frac{\partial}{\partial x_i}}\omega = dy_i.$$

The following equations hold for the Poisson bracket:

$$\{x_i, x_j\} = \{y_i, y_j\} = 0,$$
$$\{x_i, y_j\} = \delta_{ij},$$

for $1 \leq i, j \leq n$. For $H \in C^\infty(M)$ we have:

$$dH = \sum_{i=1}^n (\frac{\partial H}{\partial x_i} dx_i + \frac{\partial H}{\partial y_i} dy_i) = \iota_{X_H}\omega.$$

This implies:

$$X_H = \sum_{i=1}^n (\frac{\partial H}{\partial y_i}\frac{\partial}{\partial x_i} - \frac{\partial H}{\partial x_i}\frac{\partial}{\partial y_i}).$$

The Poisson bracket of f and g then becomes:

$$\{f, g\} = \omega(X_f, X_g) = \sum_{i=1}^n (\frac{\partial f}{\partial x_i}\frac{\partial g}{\partial y_i} - \frac{\partial f}{\partial y_i}\frac{\partial g}{\partial x_i}).$$

A curve $\rho(t) = (x_1(t), \ldots, x_n(t), y_1(t), \ldots, y_n(t))$ is an integral curve of the Hamiltonian vector field X_H with Hamiltonian H if and only if:

$$\dot{x_i} = X_H(x_i) = \frac{\partial H}{\partial y_i},$$
$$\dot{y_i} = X_H(y_i) = -\frac{\partial H}{\partial x_i},$$

for $1 \leq i \leq n$. These equations are known as the **Hamilton equations**. The Hamilton equations are always satisfied locally for an integral curve of X_H.

Remark 2.2.17. The Hamilton equations are used extensively in physics for solving problems in classical mechanics. They provide a way of calculating the trajectories of a particle in local coordinates.

Definition 2.2.18. A **Hamiltonian system** is a manifold M with a symplectic form ω and a Hamiltonian $H \in C^\infty(M)$. The system is denoted by (M, ω, H).

Definition 2.2.19. The $2n$-dimensional Hamiltonian systrem (M, ω, H) is called **completely integrable** or **integrable** if there are integrals of motion $f_1 = H, f_2, \ldots, f_n \in C^\infty(M)$ such that:

1. $f_1, \ldots, f_n$ are in **involution**, i.e. $\{f_i, f_j\} = 0$ for $1 \leq i, j \leq n$.
2. $f_1, \ldots, f_n$ are independent in the sense that $(df_1)_p, \ldots, (df_n)_p$ are linearly independent at all points $p \in D \subset M$ for some dense set D in M.

Remark 2.2.20. Every two-dimensional Hamiltonian system is trivially integrable with $f_1 = H$. Without proof we mention that every Hamiltonian system is locally integrable on some neighbourhood around a point p if $H(p) \neq 0$. The physical importance of integrability is the existence of globally conserved quantities.

2.3 Moment maps

Let G be a Lie group and $\mathfrak{g}$ its Lie algebra. In order to define moment maps, we first recall the definition of a Lie group action in order to fix some notation, and we treat some important examples.

Definition 2.3.1. A (left) **Lie group action** of G on a manifold M is a group homomorphism $\phi : G \to \mathrm{Diff}(M)$, such that the map $G \times M \to M$, $(g, m) \mapsto \phi(g)(m)$ is smooth. A manifold M with an action of G, is called a G-**manifold**.

We will sometimes write ϕ_g for $\phi(g)$.

Remark 2.3.2. Analogously, we define a right action as an anti-homomorphism. If we just say action, we mean a left action.

Definition 2.3.3. An action is called **transitive** if it has only one orbit.

Example 2.3.4. A Lie group G acts on itself in the following ways:

$$\begin{aligned} L_g : G \to G, \qquad & L_g(h) = gh, \\ R_g : G \to G, \qquad & R_g(h) = hg^{-1}, \\ \mathrm{Ad}(g) : G \to G, \qquad & \mathrm{Ad}(g)(h) = ghg^{-1}. \end{aligned}$$

It follows that $\mathrm{Ad}(g) = L_g R_g$. We call L and R the left and right action of G on itself respectively. Ad is called the **adjoint action**.

Remark 2.3.5. Ad induces an action on $\mathfrak{g}$, by abuse of notation also denoted by Ad (cf. [18]). $\mathrm{Ad}(g)(X)$ is the infinitesimal generator of the one-parameter group $g(\exp tX)g^{-1}$.

Definition 2.3.6. The **adjoint representation** ad of a Lie algebra $\mathfrak{g}$ on itself is defined by $\mathrm{ad}(X)(Y) = [X, Y]$.

Remark 2.3.7. This representation is the Lie algebra representation induced by Ad. This representation makes sense in a merely algebraic setting as well [17].

Definition 2.3.8. The **coadjoint action** Ad^* of G on $\mathfrak{g}^*$ is defined by:

$$\langle \mathrm{Ad}^*(g)\eta, Y\rangle = \langle \eta, \mathrm{Ad}(g^{-1})Y\rangle,$$

where $\langle ., .\rangle$ denotes the usual pairing of $\mathfrak{g}$ with its dual. Its infinitesimal analogue ad^*, the coadjoint action of $\mathfrak{g}$ on $\mathfrak{g}^*$ is given by:

$$\langle \mathrm{ad}^*(X)\eta, Y\rangle = \langle \eta, \mathrm{ad}(-X)Y\rangle = -\langle \eta, [X, Y]\rangle.$$

Remark 2.3.9. Note that $\omega^\eta(X, Y) := -\langle \eta, [X, Y]\rangle$ with $\eta \in \mathfrak{g}^*$ defines an antisymmetric bilinear form on $\mathfrak{g}$.

Let now (M, ω) be a symplectic manifold, G be a Lie group and $\mathfrak{g}$ its Lie algebra. $\mathfrak{g}^*$ denotes the dual vector space of $\mathfrak{g}$.

Definition 2.3.10. A (Lie group) action $\phi : G \to \mathrm{Diff}(M)$, $g \mapsto \phi_g$ is called a **symplectic action** if each ϕ_g is a symplectomorphism, i.e. if $\phi : G \to \mathrm{Sympl}(M, \omega) \subset \mathrm{Diff}(M)$.

Definition 2.3.11. A symplectic action $\phi : G \to \mathrm{Sympl}(M)$ is called a **Hamiltonian action** if there exists a map $\mu : M \to \mathfrak{g}^*$ such that for all functions $\mu^X \in C^\infty(M)$ given by $\mu^X(x) = \langle \mu(x), X\rangle$ with $X \in \mathfrak{g}$:

1. for each $X \in \mathfrak{g}$ we have $d\mu^X = \iota_{X^\sharp}\omega$, i.e. μ_X is a Hamiltonian function for the vector field $X^\sharp$, where $X^\sharp$ is the infinitesimal generator of the action corresponding to the one-parameter subgroup corresponding to X;

2. the map μ is equivariant with respect to ϕ and the coadjoint action: $\mu \circ \phi_g = Ad^*_g \circ \mu$ for all $g \in G$.

(M, ω, G, μ) is called a **Hamiltonian G-space** and μ is called a **moment map**.

Remark 2.3.12. The name moment map was used by French mathematicians and is chosen because it is a generalization of linear and angular momentum.

Remark 2.3.13. A moment map is unique up to addition of an element of $\mathfrak{g}^*$ that does not transform under Ad^*.

Example 2.3.14. The moment map on $(\mathbb{R}^{6N}, \omega_0)$, which is the phase space of N particles, with respect to the usual action of $G = \mathbb{R}^3 \rtimes \mathrm{O}(3)$, the Euclidean motion group, on $\mathbb{R}^3$, is given by

$$\mu(q, p) = \sum_{i=1}^{N} (\mathbf{p}^i, \mathbf{q}^i \times \mathbf{p}^i),$$

where $\mathbf{q}^i$ and $\mathbf{p}^i$ denote the position and the momentum of the i^{th} particle respectively.

Definition 2.3.15. An **integral of motion** of a Hamiltonian G-space (M, ω, G, μ) is a G-invariant function $f \in C^\infty(M)$. If μ is constant along the integral curves of H_f, the flow $\{\exp tH_f \mid t \in \mathbb{R}\}$ is called a **symmetry** of (M, ω, G, μ).

Theorem 2.3.16 (Noether)**.** If (M, ω, G, μ) is a Hamiltonian G-space with G connected and f is an integral of motion, then the flow of the corresponding Hamiltonian vector field X_f is a symmetry. Conversely, if the flow of some Hamiltonian vector field X_f is a symmetry, then its corresponding Hamiltonian function f is an integral of motion with respect to the G-action.

2.4 Contangent bundles

The **cotangent bundle** of a manifold was historically one of the motivating examples for the study of symplectic manifolds. Let M be an n-dimensional manifold and let $(U, x_1, \ldots, x_n)$ be a local chart. Then the differentials $(dx_i)_x$ form a basis of T_x^*M. For $y \in T_x^*M$, write $y = \sum_{i=1}^n y_i (dx_i)_x$. In this way, $(T^*U, x_1, \ldots, x_n, y_1, \ldots, y_n)$ is a local chart of T^*M, so T^*M becomes a $2n$-dimensional manifold.

Let $\pi : T^*M \to M$ be the natural projection. In coordinates, it is given by $\pi(x, y) = x$, where $x \in M$ and $y \in T_x^*M$. This induces a one-form α on T^*M by $\alpha_{(x,y)} = (d\pi_{(x,y)})^* y = y \circ d\pi_{(x,y)}$, called the **canonical one-form** on T^*M. In local coordinates $(T^*U, x_1, \ldots, x_n, y_1, \ldots, y_n)$, we have:

$$\alpha = \sum_{i=1}^n y_i dx_i.$$

We now define the **canonical symplectic form** on T^*M by $\omega = -d\alpha$. In local coordinates we have:

$$\omega = -d(\sum_{i=1}^n y_i dx_i) = \sum_{i=1}^n dx_i \wedge dy_i.$$

This two-form is nondegenerate. It is closed, because $d\omega = -d^2\alpha = 0$.

We now consider diffeomorphisms of manifolds and describe how they induce symplectomorphisms of their cotangent bundles in a natural way.

Definition 2.4.1. Let $\phi : M \to N$ be a diffeomorphism of manifolds. Let α_M and α_N be the canonical one-forms on their cotangent bundles. The **lift** $\phi_\sharp : T^*M \to T^*N$ of ϕ is a diffeomorphism defined as follows:

$$\phi_\sharp((x_1, y_1)) = (x_2, y_2),$$

where

$$\begin{aligned} x_2 &= \phi(x_1), \\ y_1 &= (d\phi_{x_1})^* y_2. \end{aligned}$$

Here, $(df_{x_1})^*$ is the inverse of $f_\sharp|_{T^*_{x_1}M}$.

Proposition 2.4.2. $\phi_\sharp$ pulls back the canonical one-form α_N to α_M, i.e. $(\phi_\sharp)^*\alpha_N = \alpha_M$.

This result is proved by calculations.

Corollary 2.4.3. The lift $\phi_\sharp : T^*M \to T^*N$ of a diffeomorphism $\phi : M \to N$ is a symplectomorphism, i.e. $(\phi_\sharp)^*\omega_2 = \omega_1$.

Corollary 2.4.4. The group $\mathrm{Diff}(M)$ of diffeomorphisms of M can be mapped to the group $\mathrm{Sympl}(T^*M, \omega)$ of symplectomorphisms of the cotangent bundle T^*M of M by $\phi \mapsto \phi_\sharp$. This map is an injective homomorphism of groups. It is not surjective.

From the following theorem, it follows that we can determine whether or not a symplectomorphism of a cotangent bundle is the lift of a diffeomorphism.

Proposition 2.4.5. A symplectomorphism $\Phi : T^*M \to T^*M$ is the lift of a diffeomorphism $\phi : M \to M$ if and only if $\Phi^*\alpha = \alpha$, where α is the canonical one-form.

Chapter 3

Spheres and hyperboloids

In this text, two spaces are of special importance: the sphere and the hyperboloid. Before introducing these spaces, we first introduce the reader to a family of groups that is of importance for the study of the symmetries of the Kepler problem, and that is closely related to the geometry of the just mentioned spaces.

3.1 Pseudo-orthogonal groups

The orthogonal group $\mathrm{O}(n+1)$ and the Lorentz group $\mathrm{O}(n,1)$, acting naturally on $\mathbb{R}^{n+1}$, turn out to be very important in the study of the Kepler problem. We assume that the reader is familiar with the orthogonal group and give some basic results about the **pseudo-orthogonal (Lie) groups** $\mathrm{O}(p,q)$ and their Lie algebras $\mathfrak{o}(p,q)$ below. The family of Lorentz groups forms a special class of pseudo-orthogonal groups, namely the class for which $q = 1$.

Consider the vector space $\mathbb{R}^{p+q} = \mathbb{R}^p \oplus \mathbb{R}^q$. Denote $w = (x, y) \in \mathbb{R}^{p+q}$ for $x \in \mathbb{R}^p$ and $y \in \mathbb{R}^q$. Without loss of generality, we assume that $p \geq q$. Define an indefinite inner product on $\mathbb{R}^{p+q}$ by:

$$\langle w_1, w_2 \rangle_{p,q} = \langle x_1, x_2 \rangle - \langle y_1, y_2 \rangle$$

where $w_1 = (x_1, y_2)$ and $w_2 = (x_2, y_2)$ and $\langle ., . \rangle$ (by abuse of notation) denotes the standard inner product. The "norm" $\|.\|_{p,q}$ of a vector $w = (x, y)$ in $\mathbb{R}^{p+q}$ induced by $\langle ., . \rangle_{p,q}$ is defined by $\|w\|_{p,q}^2 = \|x\|^2 - \|y\|^2$, where $\|.\|$ denotes the standard norm on Euclidean space. The space $(\mathbb{R}^{p+q}, \langle ., . \rangle_{p,q})$ is denoted by $\mathbb{R}^{p,q}$.

The isometry group of $\mathbb{R}^{p,q}$ with respect to $\langle ., . \rangle_{p,q}$ consists of all $g \in \mathrm{GL}(p+q, \mathbb{R})$ such that for all $w_1, w_2 \in \mathbb{R}^{p,q}$:

$$\langle g w_1, g w_2 \rangle_{p,q} = \langle w_1, w_2 \rangle_{p,q}.$$

Since $\mathrm{O}(n)$ is the group of linear isometries of $\mathbb{R}^n$ with respect to $\langle ., . \rangle$, the group $\mathrm{O}(p) \times \mathrm{O}(q)$ becomes a subgroup of $\mathrm{O}(p,q)$. This subgroup stabilizes the decomposition $\mathbb{R}^{p+q} = \mathbb{R}^p \oplus \mathbb{R}^q$. Since $\mathrm{O}(n)$ is a compact Lie group for all $n \in \mathbb{N}$, also $\mathrm{O}(p) \times \mathrm{O}(q)$

is a compact subgroup of $\mathrm{O}(p,q)$. It is actually a maximal compact subgroup, which plays an important role in the representation theory of Lie groups. However, we will focus on the Lie algebras.

The Lie algebra $\mathfrak{o}(p,q)$ of $\mathrm{O}(p,q)$ consists of the matrices $X \in M_{p+q}(\mathbb{R})$ such that $X = \rho'(0)$ for some C^∞ curve $\rho : (-\varepsilon, \varepsilon) \to \mathrm{O}(p,q)$ such that $\rho(0) = I$. We obtain

$$\mathfrak{o}(p,q) = \{X \in M_{p+q}(\mathbb{R}) | \langle Xw_1, w_2\rangle_{p,q} + \langle w_1, Xw_2\rangle_{p,q} \, \forall w_1, w_2 \in \mathbb{R}^{p+q}\}.$$

It turns out that the elements of this Lie algebra are the $(p+q) \times (p+q)$-matrices X of the form

$$X = \begin{pmatrix} A & B \\ B^T & C \end{pmatrix}$$

such that $A = -A^T \in M_p(\mathbb{R})$, $C = -C^T \in M_q(\mathbb{R})$ and $B \in M_{p,q}(\mathbb{R})$.

3.2 Riemannnian manifolds of constant curvature

We first recall the definition of a Riemannian manifold and some properties of such manifolds.

Definition 3.2.1. Let M be a manifold of dimension n. A **Riemannian metric** on M is a family of inner products g_p on the tangent spaces T_pM for $p \in M$, which depends smoothly on p, i.e. on a chart (U, x) we can write it as the form $\sum_{i,j=1}^n g_{ij} dx^i dx^j$ for every $p \in U$, where $(g_{ij}(p))$ is a positive-definite symmetric matrix for all $p \in M$ and $g_{ij} : U \to \mathbb{R}$ is smooth. A manifold with a Riemannian metric defined on it is called a **Riemannian manifold**.

Definition 3.2.2. A **Levi-Civita connection** ∇ on a Riemannian manifold (M, g) is an affine connection that is metric-preserving, i.e. $X(g(Y,Z)) = g(\nabla_X Y, Z) + g(Y, \nabla_X Z)$, and torsion-free, i.e. $\nabla_X Y - \nabla_Y X = [X, Y]$ for all vector fields X, Y, Z.

Proposition 3.2.3. A Riemannian manifold has a unique Levi-Civita connection.

Recall that the best known way of describing the curvature of a Riemannian manifold is by the Riemann curvature tensor.

Definition 3.2.4. The **Riemann curvature tensor** is the smooth tensor field $R : \mathcal{X}_M \times \mathcal{X}_M \times \mathcal{X}_M \to \mathcal{X}_M$ given by

$$R(X,Y)Z = \nabla_X \nabla_Y Z - \nabla_Y \nabla_X Z - \nabla_{[X,Y]} Z,$$

for all smooth vector fields $X, Y, Z \in \mathcal{X}_M$, the set of smooth vector fields on M, where ∇ is the Levi-Civita connection.

The Riemann curvature tensor describes the curvature of the manifold at all points. There is another notion of curvature, which only depends on the choice of a two-dimensional plane in the tangent space of a point. It is defined as a contraction of the Riemann curvature tensor.

Definition 3.2.5. Let σ be a two-dimensional subspace of T_pM with basis u, v. The **sectional curvature** of M along σ is given by

$$K(\sigma) = -\frac{g(R(u,v)u,v)}{g(u,u)g(v,v) - g(u,v)^2}$$

Definition 3.2.6. A Riemannian manifold is called **geodesically complete** or **complete** if every geodesic can be extended to a **geodesic line**, i.e. a geodesic with domain $\mathbb{R}$.

The sphere and the hyperboloid have an intrinsic geometric definition. For each $n \in \mathbb{N}$ and $k \in \mathbb{R}$ it is possible to define a simply connected n-dimensional complete Riemannian manifold M of constant sectional curvature k. For a proof of this fact, cf. [20, Theorem V.3.1]. Let n be given. We distinguish three cases:

1. For $k > 0$, the manifold M is called **elliptic**.
2. For $k < 0$, the manifold M is called **hyperbolic**.
3. For $k = 0$, the manifold M is called **flat**.

For our purposes, it is useful and sufficient to have an explicit geometric realization of these three possibilities. A realization of the n-dimensional flat Riemannian manifold is given by the n-dimensional Euclidean space. The n-dimensional elliptic Riemannian manifold of sectional curvature k can be described by the n-sphere of radius $k^{\frac{1}{2}}$. For each hyperbolic space there is an n-hyperboloid isometric to it. Because we consider spaces up to diffeomorphism, we may restrict ourselves to a realization of Riemannian manifolds of constant sectional curvature of each of the following three sectional curvatures: $k = 0$ (Euclidean space), $k = 1$ (unit sphere), $k = -1$ (unit hyperboloid). We assume that the n-Euclidean space is well-known to the reader. In the next sections, we introduce the unit sphere and the unit hyperboloid and describe some of their important properties. For more information about these manifolds, cf. [20, Section V.3] and [30]. In the rest of this text, we use the geometric realizations described below rather than the abstract definition.

3.3 Sphere

The **unit n-sphere** S^n, or **sphere** for short, consists of the points in $\mathbb{R}^{n+1}$ of modulus 1 with respect to the Euclidean norm. We thus have

$$S^n = \{x \in \mathbb{R}^{n+1} \mid \|x\| = 1\}.$$

The Euclidean distance between points on the sphere is not intrinsic to the sphere. An intrinsic notion of distance on the sphere is given by arclength. After embedding in Euclidean space, this **spherical metric** is given by

$$d_S(x,y) = \theta(x,y) = \arccos\left(\frac{\langle x, y\rangle}{\|x\|\|y\|}\right),$$

which corresponds to the Euclidean angle between the points x and y defined via the standard inner product on $\mathbb{R}^{n+1}$. The spherical metric and the Euclidean metric define the same topology on the sphere. The following theorem classifies the geodesic curves S^n.

Proposition 3.3.1. Let $\xi : [a, b] \to S^n$ be a curve such that $b - a < \pi$. Then the following statements are equivalent:

1. ξ is a geodesic curve parametrized by arc length s with respect to the spherical metric.
2. There are orthogonal vectors $x, y \in S^n$ such that $\xi(s) = \cos(s-a)x + \sin(s-a)y$.
3. The curve $\xi(s)$ satisfies $\xi'' + \xi = 0$ in $\mathbb{R}^{n+1}$.

For a proof, cf. [30], Theorem 2.1.4.

We say that the intersection of S^n with a two-dimensional linear subspace of $\mathbb{R}^{n+1}$ is a **great circle** of S^n. A consequence of Proposition 3.3.1 is that the geodesic lines[1] on S^n correspond to its great circles, in the sense that every geodesic curve can be extended to a great circle. This also explains why d_S corresponds to the notion of geodesic distance between two points on the sphere, because three points are spherically collinear, i.e. collinear with respect to d_S if they all lie on the same great circle.

Another important result we need, has to do with the symmetry of the sphere. Recall that an isometry from a metric space (X, d_X) to a metric space (Y, d_Y) is a continuous bijection that preserves the distance, i.e. ϕ is an isometry if and only if $d_Y(\phi(x), \phi(y)) = d_X(x, y)$ for all $x, y \in X$. The set of isometries of a metric space to itself form a group with respect to composition. This group is called the **isometry group**.

Proposition 3.3.2. The isometry group of the sphere S^n is isomorphic to the orthogonal group $\mathrm{O}(n + 1)$.

For a proof, cf. [30, Theorem 2.1.3]. In this way, $\mathrm{O}(n + 1)$ defines a very important symmetry group of S^n.

3.4 Hyperboloid

The hyperboloid is, like the sphere, defined as the level set of a "norm" on $\mathbb{R}^{n+1}$, but not of the Euclidean norm. The hyperboloid is embedded in the space $\mathbb{R}^{n,1}$, which was described at the start of this chapter. Its underlying space is $\mathbb{R}^{n+1}$ and it has the following indefinite inner product:

$$\langle x, y \rangle_L = x_1 y_1 + \ldots + x_n y_n - x_{n+1} y_{n+1}.$$

[1] A geodesic line is a geodesic curve with domain $\mathbb{R}$.

$\mathbb{R}^{n,1}$ is called the **Lorentzian** $(n+1)$**-space** and $\langle ., . \rangle_L$ is called the **Lorentzian inner product**.

The Lorentzian inner product defines a "norm", the **Lorentzian norm**, in the following way:

$$\|x\|_L^2 = \langle x, x \rangle_L.$$

In Lorentzian spaces there is a certain asymmetry between the different coordinates. Therefore, it makes sense to define some properties that vectors may or may not have. First we define another space.

Definition 3.4.1. The **light cone** C^n consists of the points in $\mathbb{R}^{n,1} \setminus \{0\}$ of modulus 0 with respect to the Lorentzian norm. We thus have:

$$C^n = \{x \in \mathbb{R}^{n,1} \setminus \{0\} \mid \|x\|_L = 0\}.$$

Remark 3.4.2. The name light cone is chosen, because in Einstein's special theory of relativity, which is defined in $\mathbb{R}^{3,1}$, the light cone corresponds to that part of spacetime minus the origin that would be passed by a flash of light emanating from the origin in all directions.

Definition 3.4.3. Let $x \in \mathbb{R}^{n+1}$. We say that x is **light-like** if $\|x\|_L = 0$. We say that x is **space-like** (**time-like**) if $\|x\|_L^2 > 0$ ($\|x\|_L^2 < 0$). A time-like vector x is **positive** (**negative**) if $x_{n+1} > 0$ ($x_{n+1} < 0$).

For two positive or two negative time-like vectors x, y in $\mathbb{R}^{n,1}$, there is a unique non-negative $\eta(x, y) \geq 0$ such that $\langle x, y \rangle_L = \|x\|_L \|y\|_L \cosh \eta(x, y)$. This number is called the **Lorentzian time-like angle** between x and y. We see that $\eta(x, y) = 0$ if and only if $x = \lambda y$ with $\lambda \geq 0$.

Definition 3.4.4. The **unit** n**-hyperboloid** H^n, or **hyperboloid** for short, consists of the points in $\mathbb{R}^{n,1}$ of Lorentzian norm -1 and $x_{n+1} > 0$. We thus have:

$$H^n = \{x \in \mathbb{R}^{n+1} \mid \|x\|_L^2 = -1,\ x_{n+1} > 0\}.$$

This space is, in some sense, analogous to the sphere, since it corresponds to the level set of the Lorentzian norm of imaginary unit length. However, this analogy does not hold for its topology, since S^n is compact and H^n is not. We could equally well have defined the hyperboloid as the set of points $x \in \mathbb{R}^{n+1}$ such that $\|x\|_L^2 = -1$ and $x_{n+1} < 0$, because the two spaces are homeomorphic. They both form a model of the hyperbolic space form of constant sectional curvature $k = -1$. However, we call this space H_-^n and adopt the following notation:

$$F^n = \{x \in \mathbb{R}^{n+1} | \|x\|_L^2 = -1\} = H^n \cup H_-^n.$$

We say that H^n (H_-^n) is the **positive** (**negative**) **sheet** of F^n. An intrinsic metric on H^n written after embedding in the coordinates of $\mathbb{R}^{n+1}$ is given by the **hyperbolic metric**

$$d_H(x, y) = \eta(x, y).$$

Geodesics on H^n are classified by the following theorem.

Proposition 3.4.5. Let $\xi : [a, b] \to H^n$ be a curve. Then the following statements are equivalent:

1. ξ is a geodesic curve parametrized by arc length s with respect to the hyperbolic metric.

2. There are vectors $x, y \in \mathbb{R}^{n,1}$ that are orthogonal with respect to $\langle ., . \rangle_L$ such that $\xi(s) = \cosh(s - a)x + \sinh(s - a)y$.

3. The curve $\xi(s)$ satisfies $\xi'' - \xi = 0$.

For a proof, cf. [30, Theorem 3.2.4].

We say that the intersection of H^n with a two-dimensional linear subspace of $\mathbb{R}^{n,1}$ which contains a time-like vector is a **hyperbolic line** of H^n. A consequence of Proposition 3.4.5 is that the geodesics on H^n correspond to its hyperbolic lines in the sense that every geodesic curve can be extended to a hyperbolic line. Similarly, we can define hyperbolic lines on H^n_-.

We also know the symmetry group of F^n.

Proposition 3.4.6. The group of isometries $\phi : F^n \to F^n$ is isomorphic to the Lorentz group $\mathrm{O}(n, 1)$, explicitly given by the set of matrices $T \in Mat_{n+1}(\mathbb{R})$ such that $T^t J T = J$, where $J = \mathrm{diag}(1, \ldots, 1, -1)$.

3.5 Stereographic projection

It is well-known that the n-sphere punctured at one point is topologically equivalent to $\mathbb{R}^n$. An analogue of this is true for the hyperboloid. Below we will make these statements precise.

Consider the punctured sphere, i.e. the sphere with one point removed from it. Without loss of generality we assume that this point is the north pole $N = (0, \ldots, 0, 1)$. We write $\hat{S}^n = S^n \setminus \{N\}$. Define the **spherical stereographic projection** from the north pole $\sigma : \hat{S}^n \to \mathbb{R}^n$ as the map given by

$$x_k = \frac{\xi_k}{1 - \xi_{n+1}}$$

for $k = 1, \ldots, n$. This map is smooth, because $\xi_{n+1} \neq 1$ in $\hat{S}^n$. Furthermore, it is bijective. Its inverse is given by

$$\xi_k = \frac{2x_k}{1 + \|x\|^2} \quad \text{and} \quad \xi_{n+1} = -\frac{1 - \|x\|^2}{1 + \|x\|^2}$$

for $k = 1, \ldots, n$. This map is also smooth. So the spherical stereographic projection is a diffeomorphism. Geometrically, the spherical stereographic projection assigns to a point P on $\hat{S}^n$ the point of intersection of the straight line generated by the points

P and N and the plane $\mathbb{R}^n$ through the origin perpendicular to the vector from 0 to N.

The hyperbolic analogue of the stereographic projection of the sphere is defined as follows. Consider the space $F^n := H^n \cup H^n_-$. In order to map this space to $\mathbb{R}^n$, we again remove the point $N = (0, \ldots, 0, 1)$ and write $\hat{F}^n$ for $F^n \setminus \{N\}$. The **hyperbolic stereographic projection** from the north pole is the map $\sigma : \hat{F}^n \to \mathbb{R}^n \setminus S^{n-1}$ given by

$$x_k = \frac{\xi_k}{1 - \xi_{n+1}}$$

for $k = 1, ...n$. This map is smooth, because $\xi_{n+1} \neq -1$ in $\hat{F}^n$. Furthermore, it is bijective. Its inverse is given by

$$\xi_k = \frac{2x_k}{1 - \|x\|^2} \quad \text{and} \quad \xi_{n+1} = \frac{\|x\|^2 + 1}{\|x\|^2 - 1}$$

for $k = 1, \ldots, n$. This map is also smooth. So the hyperbolic stereographic projection is a diffeomorphism. Geometrically, the hyperbolic stereographic projection assigns to a point P on $\hat{F}^n$ the point of intersection of the straight line generated by the points P and N and the plane $\mathbb{R}^n$ through the origin perpendicular to the vector from 0 to N. We can restrict the hyperbolic stereographic projection to the space $H^n \setminus \{N\}$ or H^n_-.

Remark 3.5.1. If it is clear which stereographic projection is meant, we will omit the adjectives spherical and hyperbolic.

3.6 Representation theory of $\mathfrak{o}(d,1)$

For the discussion of the symmetries of a manifold, it is useful to consider the representations of its symmetry groups. Recall that a representation of a Lie group G on a Hilbert space $\mathcal{H}$ is an action $\phi : G \to \mathcal{B}(\mathcal{H})$ such that the corresponding map $G \times \mathcal{H} \to \mathcal{H}$ is continuous and such that the image of ϕ is the set of the bounded linear operators with bounded inverse, which is a subset of $\mathcal{B}(\mathcal{H})$, the set of bounded linear operators on $\mathcal{H}$. If $\mathcal{H}$ is finite-dimensional, then ϕ is automatically smooth. Lie group representations induce representations of the corresponding Lie algebras. We will in particular look at the latter ones, since for our purposes they give enough information about the groups, and they are technically simpler.

The infinitesimal symmetries that are important for the study of the d-dimensional Kepler problem are given by the Lie algebras $\mathfrak{so}(d+1)$ and $\mathfrak{o}(d,1)$, called the **special orthogonal (Lie) algebra** and the **Lorentz (Lie) algebra** respectively. We assume that the reader is acquainted with the representation theory of the special orthogonal algebras, which is described in [14, 17]. We will explain the important aspects of the representation theory of the Lorentz algebra [14, 16].

We already introduced the light cone C^d. Denote by $C^{d,+}$ the so-called **positive light cone**, which consists of all points of the light cone for which $x_{d+1} > 0$. The **proper Lorentz group** $\mathrm{O}^\circ(d,1)$ acts transitively on $C^{d,+}$.

Definition 3.6.1. Let $s \in \mathbb{C}$. The space S_s of **homogeneous functions** on $C^{d,+}$ of degree $-s$ is defined as follows:

$$S_s := S_s(C^{d,+}) := \{f \in C^\infty(C^{p,q}) | f(tw) = t^{-s} f(w), w \in C^{d,+}, t > 0\}.$$

It is straightforward to prove that S_s is invariant under the natural action of $\mathrm{O}(p,q)$.

We consider the spaces S_s as representation spaces of $\mathfrak{o}(d,1)$ with spectral parameter s. From the theory of spherical harmonics we recall the following result, which is explicitly proved in [14].

Lemma 3.6.2.

$$S_s \cong \oplus_m H^m(\mathbb{R}^d) x_{d+1}^{-(s+m)},$$

where $H^m(\mathbb{R}^d)$ denotes the space of harmonic polynomials of degree m.

We will need the unitary irreducible representations of the Lorentz algebra in order to determine the positive spectrum of the hydrogen atom. They are classified by the following result.

Theorem 3.6.3. The space S_s is a unitary irreducible representation of the Lorentz algebra $\mathfrak{o}(d,1)$ if and only if either $\Re(s) = \frac{d-1}{2}$ or $0 < s < d-1$.

A proof of this theorem is obtained by using the decomposition of S_s as given in the previous lemma and the action of the elements of $\mathfrak{o}(d,1)$ on S_s.

Chapter 4

The Classical Kepler Problem

In this chapter, we use the mathematical concepts introduced earlier to describe the classical d-dimensional Kepler problem (for $d \geq 2$) in a rigorous way in terms of its geometry. As described in Chapter 1, the classical Kepler problem is determined by the Kepler Hamiltonian:

$$H = \frac{\|p\|^2}{2\mu} - \frac{k}{\|q\|}.$$

We do not specify any initial values or boundary conditions.

First, Kepler's laws are derived in d dimensions by means of integrals of motions and geometry. Then the Kepler orbits are related to geodesics on Riemannian manifolds of constant sectional curvature. In particular, this treatment gives rise to a regularization of the Kepler orbits, in the sense that the energy surfaces, which contain incomplete motions, are embedded into larger manifolds with a complete Hamiltonian vector field. After that, another way of regularizing the Kepler problem is described. At the end, we exhibit the relation between the two regularizations. Along the way, we also determine the symmetry group of the problem.

4.1 Kepler's laws

In a text about the Kepler problem, one should derive Kepler's laws of planetary motion, as given in Chapter 1, at least once. They were originally formulated for $H < 0$. This automatically implies that $k > 0$. We give a formulation of Kepler's laws in d dimensions, due to Önder and Verçin [27], which does not only apply to the bounded motions, but works for arbitrary H (except for the third law of course, in which the condition that the orbits are bounded is explicitly stated). However, our derivation of the laws is due to Van Haandel and Heckman [34, 35]. Their derivation, originally given in three dimensions, is intuitive and elegant.

Consider a particle with Hamiltonian H equal to the Kepler Hamiltonian. The d-dimensional Kepler laws are as follows:

1. the orbit of the object is a two-dimensional conic section with 0 as one of its foci;

2. the line connecting the object to 0 sweeps out equal areas in the plane of motion in equal intervals of time;

3. in the case of bounded orbits, in which the orbit is an ellipse, the period of the object is proportional to the cube of the semi-major axis of its orbit.

We will now derive these laws. To this end, we first look at some physical quantities and prove that they are integrals of motion.

The phase space of the d-dimensional Kepler problem is $T^*(\mathbb{R}^d \setminus \{0\})$, which is identified with the subspace of $(\mathbb{R}^{2d}, \omega)$ given by $\{(q,p) \in \mathbb{R}^d \oplus \mathbb{R}^d \,|\, q \neq 0\}$. The symplectic form ω is given by $\omega = \omega_0 = \sum_{i=1}^d dq_i \wedge dp_i$.

Definition 4.1.1. The **(generalized) angular momentum** L is an anti-symmetric $d \times d$-matrix given by its components

$$L_{ij} = q_i p_j - q_j p_i,$$

with $1 \leq i, j \leq d$. The **(generalized) Runge-Lenz vector** K is given by its

$$K_i = \sum_{j=1}^{d} L_{ij} p_j - \mu k \frac{q_i}{\|q\|} = \|p\|^2 q_i - \langle q, p \rangle p_i - \mu k \frac{q_i}{\|q\|},$$

with $1 \leq i \leq d$.

Remark 4.1.2. The generalized angular momentum is not an d-vector any more: it is an anti-symmetric matrix. Note that in the case $d = 3$, the usual components of L, i.e. L_1, L_2 and L_3 correspond to the matrix entries L_{23}, L_{31} and L_{12} respectively. The generalized Runge-Lenz vector indeed generalizes the usual Runge-Lenz vector, because of the three-dimensional relation $\mathbf{p} \times (\mathbf{q} \times \mathbf{p}) = \langle \mathbf{p}, \mathbf{p} \rangle \mathbf{q} - \langle \mathbf{q}, \mathbf{p} \rangle \mathbf{p}$.

First, we prove that the energy of an object with Hamiltonian H is conserved. This is however not only true for the Kepler Hamiltonian, but for more general ones.

Proposition 4.1.3. For a spherically symmetric central force field $F(q) = f(\|q\|)\frac{q}{\|q\|}$, the Hamiltonian $H = \frac{\|p\|^2}{2\mu} + V(\|q\|)$, where $V(\|q\|) = -\int f(s)ds$, is a conserved quantity.

Proof. The proof follows by explicit calculation. First note that:

$$\dot{\|q\|} = \frac{d}{dt}(\langle q, q \rangle)^{\frac{1}{2}} = \langle \dot{q}, \frac{q}{\|q\|} \rangle.$$

Hence:

$$\begin{aligned} \frac{d}{dt} H &= \frac{\langle \dot{p}, p \rangle}{\mu} + \dot{V} \\ &= \langle F, \dot{q} \rangle - f(\|q\|)\dot{\|q\|} \\ &= \langle F, \dot{q} \rangle - f(\|q\|)\langle \dot{q}, \frac{q}{\|q\|} \rangle = 0, \end{aligned}$$

because $F(q) = f(\|q\|)\frac{q}{\|q\|}$. ∎

Corollary 4.1.4. The Kepler Hamiltonian is conserved.

Proposition 4.1.5. The angular momentum $L = (L_{ij})$ and the Runge-Lenz vector $K = (K_i)$ are integrals of motion.

Proof. For all $i, j \in \{1, \dots, d\}$ we have:

$$\begin{aligned}\{H, L_{ij}\} &= \sum_{l=1}^{d} \left(\frac{\partial H}{\partial q_l} \frac{\partial L_{ij}}{\partial p_l} - \frac{\partial H}{\partial p_l} \frac{\partial L_{ij}}{\partial q_l} \right) \\ &= \sum_{l=1}^{d} \left(\frac{k}{\|q\|^3} q_l (\delta_{jl} q_i - \delta_{il} q_j) - \frac{p_l}{\mu} (\delta_{il} p_j - \delta_{jl} p_i) \right) \\ &= \frac{k}{\|q\|^3} q_j q_i - \frac{k}{\|q\|^3} q_i q_j - \frac{p_i}{\mu} p_j + \frac{p_j}{\mu} p_i = 0.\end{aligned}$$

Using this result, for all $i \in \{1, \dots, d\}$ we obtain:

$$\begin{aligned}\{H, K_i\} &= \sum_{j=1}^{d} (\{H, L_{ij}\} p_j + L_{ij} \{H, p_j\}) - \mu k \{H, \frac{q_i}{\|q\|}\} \\ &= \sum_{j=1}^{d} (q_i p_j - q_j p_i) \frac{\partial H}{\partial q_j} + \mu k \sum_{l=1}^{d} \frac{p_l}{\mu} \left(\delta_{il} \frac{1}{\|q\|} - \frac{q_i q_l}{\|q\|^3} \right) \\ &= \sum_{j=1}^{d} \left(q_i q_j p_j \frac{k}{\|q\|^3} - q_j q_j p_i \frac{k}{\|q\|^3} \right) + \sum_{l=1}^{d} \frac{p_l}{\mu} \left(\delta_{il} \frac{1}{\|q\|} - \frac{q_i q_l}{\|q\|^3} \right) \\ &= \frac{k}{\|q\|^3} \langle q, p \rangle q_i - \frac{k}{\|q\|} p_i + \frac{k}{\|q\|} p_i - \frac{k}{\|q\|^3} \langle q, p \rangle q_i = 0.\end{aligned}$$

□

Remark 4.1.6. This proposition also follow from Noether's Theorem, which is stated in this text as Theorem 2.3.16.

Corollary 4.1.7. The orbit in $\mathbb{R}^d$ of a particle described by the Kepler Hamiltonian is contained in a two-dimensional plane.

Proof. $K(t)$ is perpendicular to the plane of motion for fixed time t, since this plane is spanned by $q(t)$ and $p(t)$. Since K is an integral of motion, this plane stays the same. □

With this in mind, we can prove Kepler's second law. We assume that the plane of motion is spanned by two orthogonal unit vectors e_1 and e_2. We will write the relevant quantities with respect to this basis. In fact, all vectors are d-dimensional, but we will treat them as if they are two-dimensional.

Theorem 4.1.8. If an object subdued to a spherically symmetric central force field moves through a curve $q(t)$ in $\mathbb{R}^2$, then the area swept out by the line piece $[0, q(t)]$ per unit of time is constant.

Proof. The area A_{t_1,t_2} swept out by $[0, q(s)]$ for $t_1 \leq s \leq t_2$ for some t_1 and t_2 can be calculated by:

$$A_{t_1,t_2} = \int_{t_1}^{t_2} \frac{1}{2}\|q(t) \times \dot{q}(t)\|dt = \frac{1}{2\mu}\|l\|(t_2 - t_1), \tag{4.1}$$

where $|l|$ denotes the norm of the ordinary angular momentum of the motion in the plane, which is conserved by Proposition 4.1.5. This expression only depends on the duration $t_2 - t_1$, which proves the claim. □

Remark 4.1.9. For both claims of this proof the conservation of angular momentum has been used. The above theorem proves Kepler's second law.

Now the first law will be proved. We consider the different signs of the Hamiltonian separately. Again, note that in fact we should first distinguish between the signs of k, because a sign of k comes with the definition of the Hamiltonian itself already. Later, we summarize the results in what we call Kepler's first law. This way is chosen, because it both gives the explicit nature of the Kepler orbits for negative, positive and zero energy, and it unifies these observations into one clear statement. We consider the orbits restricted to the plane of motion.

Suppose that $H < 0$. This implies that $k > 0$.

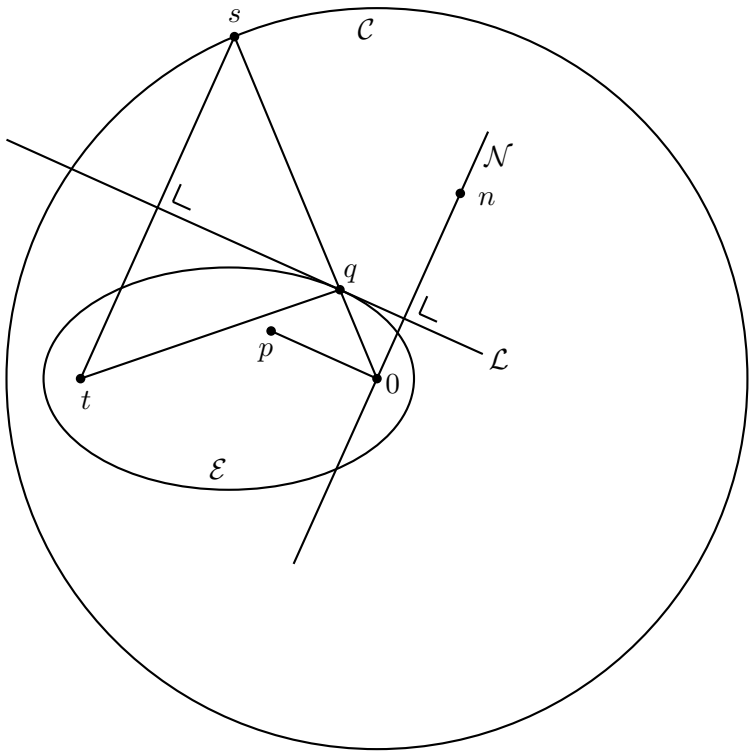
Proposition 4.1.10. The motion of the particle is bounded inside the circle (in the plane of motion) with center 0 and radius $-\frac{k}{H}$.

Proof. We have

$$-H = -\frac{\|p\|^2}{2\mu} + \frac{k}{\|q\|} \leq \frac{k}{\|q\|},$$

which implies that $\|q\| \leq -\frac{k}{H}$. So the motion takes place in the circle (in the plane of motion) with center 0 and radius $-\frac{k}{H}$. □

Consider the circle $\mathcal{C}$ centered at 0 with radius $-\frac{k}{H}$, i.e. the circle from the previous proposition. Let $s = -\frac{kq}{\|q\|H}$ be the point of intersection of the line through 0 and q and $\mathcal{C}$. The line $\mathcal{L}$ through q parallel to p is the tangent line to the orbit at the point q. Let t be the reflection of s in $\mathcal{L}$. The situation is sketched below. Note that q is on the line piece $[0, s]$.



We want to define a vector n perpendicular to p. Let us define n by

$$n = \left(q_1 p_2^2 - q_2 p_1 p_2, q_2 p_1^2 - q_1 p_1 p_2\right).$$

Indeed:

$$\langle p, n\rangle = q_1 p_1 p_2^2 - q_2 p_1^2 p_2 + q_2 p_1^2 p_2 - q_1 p_1 p_2^2 = 0.$$

Proposition 4.1.11. The point t is equal to $\frac{K}{\mu H}$.

Proof. The point t is given by:

$$t = s - 2\frac{\langle (s-q), n\rangle}{\|n\|^2} n.$$

First observe that:

$$\|n\|^2 = \|p\|^2 L_{12}^2 = \|p\|^2 (q_1 p_2 - q_2 p_1)^2.$$

We thus have:

$$\begin{aligned}
\langle (q-s), n\rangle &= \langle q + \frac{kq}{\|q\|H}, n\rangle \\
&= \left(1 + \frac{k}{\|q\|H}\right) \langle q, n\rangle \\
&= \left(1 + \frac{k}{\|q\|H}\right) \left(q_1^2 p_2^2 - q_1 q_2 p_1 p_2 + q_2^2 p_1^2 - q_1 q_2 p_1 p_2\right) \\
&= \left(1 + \frac{k}{\|q\|H}\right) \left(q_1 p_2 - q_2 p_1\right)^2.
\end{aligned}$$

Hence:

$$\begin{aligned}\mu H t &= -\mu k \frac{q}{\|q\|} + \mu H \frac{2}{\|p\|^2}\left(1 + \frac{k}{\|q\|H}\right)\left(q_1 p_2^2 - q_2 p_1 p_2, q_2 p_1^2 - q_1 p_1 p_2\right) \\ &= -\mu k \frac{q}{\|q\|} + n \\ &= K,\end{aligned}$$

using the fact that $\|p\|^2 = 2\mu(H + \frac{k}{\|q\|})$ and the form of n. □

Because the vector K is conserved, we know that t is a fixed point in space.

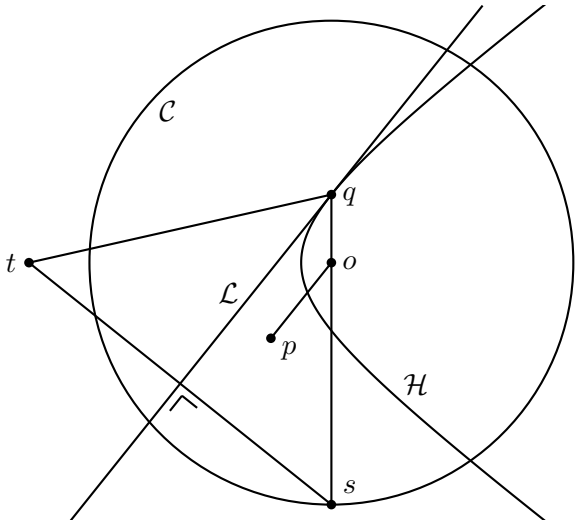
Theorem 4.1.12. The orbit of the particle is an ellipse with foci 0 and t and major axis $2a = -\frac{k}{H}$.

Proof. For a point q on the orbit we have:

$$\|q - 0\| + \|q - t\| = \|q\| + \|q - s\| = 2a.$$

This exactly characterizes an ellipse. □

Until now, we only considered the case for which $H < 0$ (and hence $k > 0$), which physically corresponds to bounded orbits. In the case that $H > 0$, it is still true that the point t is a fixed point in $\mathbb{R}^d$, since the Runge-Lenz vector is still conserved. However, the motion is not necessarily bounded to some region, as was the case for $H < 0$. In this case, the coupling constant can assign both positive and negative values. For $k > 0$, we get the situation as indicated in the figure below. Note that 0 is on the line piece $[q, s]$.



Theorem 4.1.13. Suppose that $H > 0$ and $k > 0$. The orbit of the particle is the branch of the hyperbola with foci 0 and t closest to 0 and major axis equal to $2a = \frac{k}{H}$.

Proof. We have:

$$\|q-t\| - \|q-0\| = \|q-s\| - \|q\| = \frac{k}{H}.$$

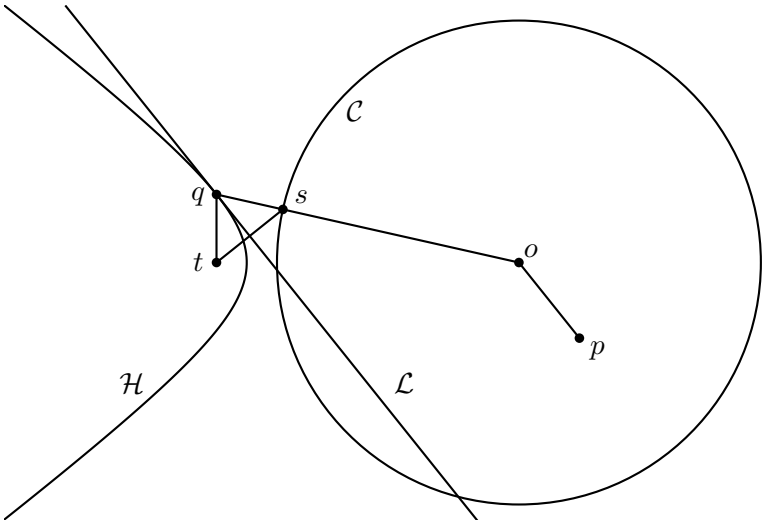
This exactly characterizes the particular hyperbola branch. □

For the case in which $H > 0$ and $k < 0$, we know that s is on the line piece $[0, q]$. We now prove a result analogous to 4.1.10.

Proposition 4.1.14. The motion of the particle in the plane of motion is outside the circle with center 0 and radius $-\frac{k}{H}$.

Proof. We have $H = \frac{\|p\|^2}{2\mu} - \frac{k}{\|q\|} \geq -\frac{k}{\|q\|}$, which implies that $\|q\| \geq -\frac{k}{H}$. □

We have the situation as sketched below.



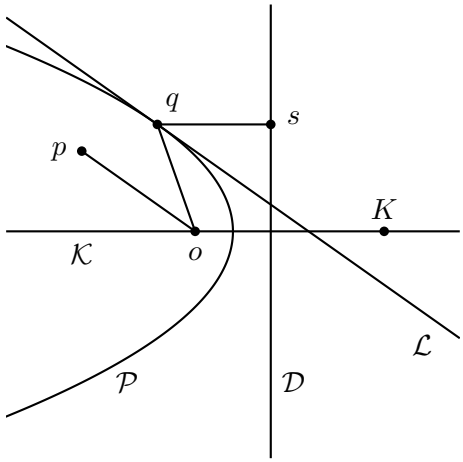
Theorem 4.1.15. Suppose that $H > 0$ and $k < 0$. The orbit of the particle is the branch of the hyperbola with foci 0 and t closest to t and major axis equal to $2a = -\frac{k}{H}$.

Proof. We have:

$$\|q-0\| - \|q-t\| = \|q\| - \|q-s\| = -\frac{k}{H}.$$

This exactly characterizes the particular hyperbola branch. □

The last case, in which $H = 0$ and hence $\|p\|^2 = \frac{2\mu k}{\|q\|}$, is sketched below. It may be the case that $k = 0$. Then the particle is free and moves along a straight line in the plane of motion. Consider now the other possible case, namely $k > 0$. Note that we now also may divide by $\|p\|$. We again define the line $\mathcal{L}$ to be the line through q tangent to the orbit. So it is parallel to p. The point s is the reflection of 0 in $\mathcal{L}$.



Proposition 4.1.16. For the point s we have $s = \frac{\|q\|}{k\mu}n$, where n is as defined above. We conclude that $s - q = \frac{\|q\|}{k\mu}K$.

Proof. s is equal to $2\frac{\langle q,n\rangle}{|n|^2}n$, which equals

$$\frac{2}{\|p\|^2}n = \frac{\|q\|}{k\mu}n,$$

using the calculations done earlier. From this, it follows that $s - q = \frac{\|q\|}{k\mu}K$. □

Theorem 4.1.17. If $H = 0$, then the orbit is the parabola with focus 0 and directrix $\mathcal{D}$.

Proof. Indeed, $\|q - s\|^2 = \|q\|^2 + \|s\|^2 - 2\langle q, n\rangle = \|q\|^2 + \frac{4}{\|p\|^4}\|n\|^2 - \frac{4}{\|p^2\|}\frac{\|n\|^2}{\|p\|^2} = \|q\|^2$, which proves the claim, because a parabola is the locus consisting of points such that the distance to a given point (its focus) and a given line (its directrix) is equal. □

We have now considered all possible cases of Kepler orbits and summarize them in the first law.

Theorem 4.1.18. The orbit of the object is a conic section with a fixed two-dimensional linear subspace with 0 as one of its foci.

Proof. The ellipse, hyperbola and parabola are the (only) two-dimensional conic sections in $\mathbb{R}^d$. □

We did not explicitly treat the degenerate conics, such as the double line, because they all are special cases of one of the above. They correspond to incomplete Kepler orbits, which will be explained in the next section.

Kepler's third law follows from the values of the parameters of the ellipse. We know that $a = -\frac{k}{2H}$. The distance $2c$ between the two foci is given by $4c^2 = \langle t, t\rangle = \frac{\|K\|^2}{\mu^2 H^2} =$

$\frac{2\mu H\|l\|^2+\mu^2k^2}{\mu^2H^2}$. Therefore the semiminor axis b of the ellipse is given by $4b^2 = -\frac{2\|l\|^2}{\mu H}$. Hence, the square of the area of this ellipse is:

$$\pi^2a^2b^2 = \pi^2\frac{k^2\|l\|^2}{8\mu H^3} = \frac{\|l\|^2T^2}{4\mu^2},$$

where T is the period of the orbit. The last expression follows from Kepler's second law. Using the relation $a = -\frac{k}{2H}$, we obtain:

$$\frac{T^2}{a^3} = \frac{4\pi^2\mu}{k} = \frac{4\pi^2}{G(m_1+m_2)},$$

which is exactly Kepler's third law. In the unified point of view, Kepler's third law is merely a special case of the second law. It relates the period of the orbit, which exists if the orbit is closed, to the semi-major axis.

4.2 Incomplete Kepler orbits

The orbits corresponding to the nondegenerate conic sections in $\mathbb{R}^d$ are regular in the sense that they correspond to a globally defined integral curve of the Hamiltonian vector field. The following result gives the intrinsic incompleteness of the Kepler problem. The degenerate conic sections in $\mathbb{R}^d$ correspond to integral curves of the Hamiltonian vector field that are not globally defined.

Proposition 4.2.1. The Kepler Hamiltonian vector field is incomplete.

Proof. Consider the motion of a particle with energy $H < 0$ and $L = 0$, i.e. this particle is on some fall circle $\mathcal{C}$ as defined in the last section. Suppose that $(q(0), \dot{q}(0)) = (-\frac{k\mu}{H}, 0)$. The time for the particle to reach the origin with infinite speed is given by:

$$T = \int_0^{-\frac{k\mu}{H}} \frac{dr}{(\frac{2k\mu}{r}+2\mu H)^{\frac{1}{2}}} < \infty,$$

so the particle gets to the origin in a finite time, which proves the proposition. □

Definition 4.2.2. The motions "through" the origin are the **incomplete motions**.

By an embedding of the incomplete phase space in another manifold with a complete Hamiltonian vector field, it can be realized that the phase space is regularized in the sense that the integral curves of the (incomplete) phase space become complete under the embedding. This process is called **regularization**. In the rest of this chapter, we will discuss two ways of **regularization** of the Kepler problem and describe how they are related.

4.3 Kepler orbits and geodesics on manifolds

We show that the space of Kepler orbits in $\mathbb{R}^d$ of a fixed energy E can be embedded in the set of geodesics on some complete Riemannian manifold of constant sectional curvature in such a way that the Hamiltonian vector field of the Kepler problem is regularized, in the sense that it is extended in such a way that the incomplete Kepler orbits are also mapped to particular geodesics. This map turns out to preserve some of the symplectic structure, but it is weaker than a symplectomorphism. Whether the manifold is of positive or negative curvature is determined by the sign of E. The method used here fits in our general method of interchanging the coordinates of position and momentum and afterwards applying a stereographic projection.

Because of the symmetry of the set of geodesics on a manifold, we will find a symmetry group along the way that is richer than the intuitively obvious symmetry group $\mathrm{O}(d)$ of the Kepler Hamiltonian.

The results in this section are due to Moser [24], but also [22, 28, 33] discuss the geometry of the phase space of the Kepler problem. [22, 28] even consider the case $E > 0$. Moser only considers the case $E < 0$, but we extend his way of reasoning to positive energies. In [22], the phase space of the Kepler problem is regularized at once, without the restriction to the energy surfaces. We will come back to this later.

The **configuration space** Q of the Kepler problem is the set of possible positions, so in the case of the d-dimensional problem, it is $\mathbb{R}^d \setminus \{0\}$. The **phase space** P is given by the cotangent bundle $T^*Q \subset \mathbb{R}^d \oplus \mathbb{R}^d$ of Q. For any $E \in \mathbb{R}$, we define the **energy surface** Σ_E of energy E to be defined by:

$$\Sigma_E := \{x \in T^*Q \mid H(x) = E\}.$$

Since the energy is conserved, these submanifolds are well-defined and closed. We introduce two open submanifolds of P as follows:

$$P_+ := \cup_{E>0}\Sigma_E,$$
$$P_- := \cup_{E<0}\Sigma_E.$$

P_+ corresponds to hyperbolic Kepler orbits, whereas P_- contains the elliptic Kepler orbits. Thus $P = P_+ \cup \Sigma_0 \cup P_-$.

In the next subsections, we map each Σ_E to the cotangent bundle of some Riemannian manifold. Hereto, we consider the cases of negative and positive energies separately. We will see that the regularization map is geometrically very simple.

4.3.1 Negative energies

Suppose $E < 0$. As described earlier, the trajectory of a particle with this Hamiltonian is an ellipse with the origin as one of its foci. Its semi-major axis a equals $-\frac{k}{2H}$.

It turns out that the elliptic Kepler orbits in d dimensions are equivalent to the geodesics on a d-sphere in a certain way. Without loss of generality, we assume that $\mu = 1$ and $k = 1$. In $\mathbb{R}^{d+1}$ we write $N = (0, \ldots, 0, 1)$.

Theorem 4.3.1. The space Σ_E of Kepler orbits with energy $E < 0$ is mapped to the unit cotangent bundle $T_1^*(\hat{S}^d)$ of $\hat{S}^d = S^d \setminus \{N\}$ by an extension of the stereographic projection in a diffeomorphic way such that the canonical one-forms match.

Proof. The sphere S^d consists of the points $\xi = (\xi_1, \ldots, \xi_{d+1}) \in \mathbb{R}^{d+1}$ for which $\|\xi\|^2 = 1$. By the stereographic projection, the sphere punctured at its north pole $N = (0, \ldots, 0, 1)$, can be mapped diffeomorphically onto $\mathbb{R}^d$, as is described in Section 3.5. We start with the geodesic flow on the sphere and map it to the space of Kepler orbits with energy $E = -\frac{1}{2}$.

A curve $\xi(s)$ on the sphere is a geodesic if and only if it satisfies:[1]

$$\xi'' + \|\xi'\|^2 \xi = 0.$$

If $\|\xi'\| = 1$, then this equation corresponds to the parametrization by arc length, which we assume from now on. If we introduce the tangent vector $\eta = \xi'$, then we have the following equations:

$$\xi' = \eta, \qquad \eta' = -\|\eta\|^2 \xi,$$

with $\|\xi\| = 1$ and $\langle \xi, \eta \rangle = 0$, since a tangent vector to the sphere are always perpendicular to the position vector of the point at which it is defined. These two equations represent the tangent bundle $T(S^d)$ of S^d, which we linearly identify with the cotangent bundle $T^*(S^d)$.

We now map the punctured sphere $\hat{S}^d$ onto $\mathbb{R}^d$ by the spherical stereographic projection and extend it to a map from $T_1^*(\hat{S}^d)$ to $T^*(\mathbb{R}^d)$ as follows. First we consider $T_1^*(\hat{S}^n)$ as a submanifold of $T^*(\mathbb{R}^{d+1})$, which we in turn identify with $\mathbb{R}^{d+1} \oplus \mathbb{R}^{d+1}$. In this embedding, $T_1^*(\hat{S}^d)$ corresponds to the pairs (ξ, η) such that $\|\xi\| = 1$, $\langle \xi, \eta \rangle = 0$ and $\|\eta\| = 1$. The canonical one-form $\theta_{\hat{S}^d}$ is the restriction of the canonical one-form on $T^*(\mathbb{R}^{d+1})$. We define the extended mapping by the following two equations:

$$\begin{aligned} x_k &= \frac{\xi_k}{1 - \xi_{d+1}}, \\ y_k &= (1 - \xi_{d+1})\eta_k + \xi_k \eta_{d+1}, \end{aligned}$$

for $k = 1, \ldots, d$. Its inverse is given by:

$$\begin{aligned} \xi_k &= \frac{2x_k}{\|x\|^2 + 1}, \\ \xi_{d+1} &= \frac{\|x\|^2 - 1}{\|x\|^2 + 1}, \\ \eta_k &= \frac{\|x\|^2 + 1}{2} y_k - \langle x, y \rangle x_k, \\ \eta_{d+1} &= \langle x, y \rangle, \end{aligned}$$

for $k = 1, \ldots, d$.

These equations define a diffeomorphism. Let us check that the canonical one-forms $\theta_{\hat{S}^d}$ and $\theta_{\mathbb{R}^d}$ are mapped to each other.[2] The canonical one-forms on $T^*\hat{S}^d$ and $T^*\mathbb{R}^d$

[1] Cf. Chapter 3.

[2] Note that $T_1^*\hat{S}^d$ is not a symplectic manifold, since it is not even-dimensional.

are given by $\theta_{\hat{S}^d} = \langle \eta, d\xi \rangle$ and $\theta_{\mathbb{R}^d} = \langle y, dx \rangle$ respectively.

If we substitute $dx_k = \frac{d\xi_k}{1-\xi_{d+1}} + \frac{d\xi_{d+1}}{(1-\xi_{d+1})^2}\xi_k$, we get

$$\begin{aligned}
\langle y, dx \rangle &= \sum_{k=1}^{d} y_k dx_k \\
&= \sum_{k=1}^{d} ((1-\xi_{d+1})\eta_k + \eta_{d+1}\xi_k) \left(\frac{d\xi_k}{1-\xi_{d+1}} + \frac{d\xi_{d+1}}{(1-\xi_{d+1})^2}\xi_k \right) \\
&= \sum_{k=1}^{d} \left(\eta_k d\xi_k + \frac{\eta_{d+1}}{1-\xi_{d+1}}\xi_k d\xi_k + \frac{\eta_k \xi_k d\xi_{d+1}}{1-\xi_{d+1}} + \eta_{d+1}\xi_k^2 \frac{d\xi_{d+1}}{(1-\xi_{d+1})^2} \right).
\end{aligned}$$

Using $0 = \frac{1}{2} d\|\xi\|^2 = \langle \xi, d\xi \rangle = \sum_{k=1}^{d} \xi_k d\xi_k + \xi_{d+1} d\xi_{d+1}$ in the second term and using the definition of the stereographic projection and the description of $T^*(S^d)$ as subspace of $\mathbb{R}^{d+1} \oplus \mathbb{R}^{d+1}$ gives us:

$$\begin{aligned}
&\sum_{k=1}^{d} \left(\eta_k d\xi_k + \frac{\eta_{d+1}}{1-\xi_{d+1}}\xi_k d\xi_k + \frac{\eta_k \xi_k d\xi_{d+1}}{1-\xi_{d+1}} + \eta_{d+1}\xi_k^2 \frac{d\xi_{d+1}}{(1-\xi_{d+1})^2} \right) \\
&= \sum_{k=1}^{d} \left(\eta_k d\xi_k - \frac{\eta_{d+1}}{1-\xi_{d+1}}\xi_{d+1} d\xi_{d+1} + \frac{-\eta_{d+1}\xi_{d+1} d\xi_{d+1}}{1-\xi_{d+1}} + \eta_{d+1} d\xi_{d+1} \right) \\
&= \langle \eta, d\xi \rangle.
\end{aligned}$$

Note that $\|\eta\| = \frac{(\|x\|^2+1)\|y\|}{2}$. The Hamiltonian of the geodesic flow is given by the Hamiltonian $\Phi(\xi, \eta) = \frac{1}{2}\|\eta\|^2$. In this way we get the following Hamiltonian in the (x, y)-space:

$$F(x, y) = \Phi(\xi, \eta) = \frac{1}{2}\|\eta\|^2 = \frac{(\|x\|^2+1)^2\|y\|^2}{8},$$

which gives the following transformed Hamilton differential equations:

$$x' = F_y, \qquad y' = -F_x. \tag{4.2}$$

This set of equations follows from straightforward calculations. The geodesics such that $\|\eta\| = 1$, and hence $\Phi = \frac{1}{2}$, correspond to solutions for which $F = \frac{1}{2}$.

Now comes the elegant part of the argument. The differential equations (4.2) form a system, in which only the first partial derivatives of F occur. We can therefore replace F by $G := u(F) := \sqrt{2F} - 1$, because this defines a differentiable function at the point $F = \frac{1}{2}$ and $u'(\frac{1}{2}) = 1$. So at this point, the gradients of both functions agree, such that:

$$x' = G_y, \qquad y' = -G_x. \tag{4.3}$$

Note that the system given by equation (4.2) with $F = \frac{1}{2}$ is mapped to the system given by equation (4.3) with $G = 0$. If we change the variable s to:

$$t = \int \|y\| ds,$$

then (denoting differentiation with respect to t by a dot) we obtain[3] $\dot{x} = \|y\|^{-1}x' = \|y\|^{-1}G_y$ and $\dot{y} = \|y\|^{-1}y' = -\|y\|^{-1}G_x$. If we define the following Hamiltonian:

$$H = \frac{1}{2}\|x\|^2 - \frac{1}{\|y\|} = \|y\|^{-1}(\sqrt{2F} - 1) - \frac{1}{2} = \|y\|^{-1}G - \frac{1}{2},$$

then we obtain the Hamilton equations $\dot{y} = H_x$ and $\dot{x} = -H_y$. So the Hamiltonian system (4.3) for $G = 0$ is mapped to this system with $H = -\frac{1}{2}$. It is obvious that after applying the canonical transformation $p = x$ and $q = -y$, the system goes over into the Kepler problem. The trajectories of the geodesic flow on the sphere away from the north pole parametrized by s are mapped to the trajectories of the Hamiltonian flow of $H = \frac{1}{2}\|x\|^2 - \frac{1}{\|y\|}$ away from $y \neq 0$ parametrized by t.

By rescaling, the energy surface corresponding to $E = -\frac{1}{2\rho^2}$ can be mapped to $T_1^*(\hat{S}^n)$ as follows:

$$q' = \rho^2 q, \qquad p' = \rho^{-1}p, \qquad t' = \rho^3 t.$$

This mapping maps the Kepler problem to itself and replaces E by $E' = \rho^{-2}E$. □

So far we have proven that any energy surface (after an appropriate rescaling) can be mapped to $T_1^*(\hat{S}^d)$ in a canonical way. We also saw that the mapping that achieves this is a diffeomorphism. By restoring the north pole, we obtain the compactification $T_1^*(S^d)$ of $T_1^*(\hat{S}^d)$. If we apply the inverse stereographic projection and the canonical interchange of the position and the momentum coordinates, the geodesics through the north pole correspond to the incomplete Kepler orbits. In this way, we also obtain a compatification $\tilde{\Sigma}_E$ of the energy surface Σ_E. Hence we obtain a regularization of the Kepler problem, since the Hamilton vector field on the unit cotangent bundle of the sphere is complete. The reparametrization of the time is essential for this regularization.

Remark 4.3.2. The formulas for the extended stereographic projection do not only make sense for energy $H = -\frac{1}{2}$ and covectors of length one. Indeed, they define a canonical map from $T^*(\hat{S}^d)$ to $T^*(\mathbb{R}^d)$. We will call the inverse of this map composed with the canonical interchange of the position and the momentum coordinates the **Moser map** Φ_M.

Remark 4.3.3. Geometrically, the north pole corresponds to the points at infinity in p-space, as can be seen from the geometry of the usual (non-extended) stereographic projection. In order to maintain a finite energy, it also corresponds to $q = 0$. The corresponding orbits are degenerated ellipses, the collision orbits of the Kepler problem. A particle moves to the origin in a straight line in a finite interval of s. After that, its motion is reflected in both position and momentum.

Corollary 4.3.4. For each $E < 0$, the regularized energy surface $\tilde{\Sigma}_E$ possesses $\mathrm{O}(d+1)$ symmetry, since this group acts on it. The energy surfaces possesses the infinitesimal symmetry $\mathfrak{so}(d+1)$.

[3]Note that $\|y\| \neq 0$, because we chose $\|\eta\| = 1$.

Proof. The group $\mathrm{O}(d+1)$ acts on the space $T_1^*(S^d)$ by matrix multiplication and takes geodesics (parametrized by arc length) into geodesics (parametrized by arc length). □

We will now derive the explicit map relating s and t. By an orthogonal transformation that leaves the ξ_{d+1}-axis invariant, we can always map a geodesic into the two-dimensional space given by $\xi_3 = \xi_4 = \xi_d = 0$. We may therefore, in what follows, assume that $d = 2$. After a suitable rotation of the geodesic [24], we have:

$$\begin{aligned}
\xi_1 &= \sin s, \\
\xi_2 &= -\cos\alpha\cos s, \\
\xi_{d+1} &= \sin\alpha\cos s, \\
\eta_k &= \xi_k',
\end{aligned}$$

for $k = 1, 2, d+1$. Here, α denotes the angle between the subspace given by $\xi_{d+1} = 0$ and the circle. The image of this circle in the (x, y)-space is:

$$\begin{aligned}
x_1 &= (1 - \sin\alpha\cos s)^{-1}\sin s, \\
x_2 &= -(1 - \sin\alpha\cos s)^{-1}\cos\alpha\cos s, \\
y_1 &= \cos s - \sin\alpha, \\
y_2 &= \cos\alpha\sin s.
\end{aligned}$$

Hence we obtain:

$$\begin{aligned}
q_1 &= -\cos s + e, \\
q_2 &= -\sqrt{1 - e^2}\sin s,
\end{aligned}$$

where $e := \sin\alpha$. This denotes an ellipse in terms of its **eccentric anomaly** s [7, 13]. t is called the **mean anomaly**. We have $\|y\| = 1 - \sin\alpha\sin s = 1 - e\cos s$. We now obtain the following expression for the rescaled time t:

$$t = \int_0^s \|y\| ds = s - e\sin s. \tag{4.4}$$

This equation is called the **Kepler equation**.

4.3.2 Positive energies

Suppose $E > 0$. Then k can either be positive or negative. The trajectory of the particle is now an arc of an hyperbola. As we saw before, which specific arc it is depends on the sign of k. Without loss of generality, we assume that $\mu = 1$ and $k = \pm 1$.

It turns out that the hyperbolic Kepler orbits are equivalent to the geodesics on a hyperboloid in a canonical way, as can be concluded by applying the same method that Moser used.

Theorem 4.3.5. The space Σ_E of Kepler orbits with energy E is mapped to the unit cotangent bundle $T_1^*(\hat{F}^d)$ of $\hat{F}^d = F^d \setminus \{N\}$ by an extension of the stereographic projection in a diffeomorphic way such that the canonical one-forms match.

The proof of this theorem is a translation of the proof of the negative energy case to the hyperbolic setting. It was suggested in the literature to do this. To my knowledge, it was first done explicitly by Adriaan Kleinhout [19].

Proof. The hyperboloid F^d consists of the points $\xi = (\xi_1, \ldots, \xi_{d+1}) \in \mathbb{R}^{d+1}$ for which $\|\xi\|_L^2 = -1$. By the stereographic projection, the hyperboloid with its north pole $N = (0, \ldots, 0, 1)$ removed can be mapped diffeomorphically onto $\mathbb{R}^d \backslash S^{d-1}$, as described in Section 3.5.

We start with the geodesic flow on the hyperboloid and map it to the space of Kepler orbits with energy $H = \frac{1}{2}$.

A curve $\xi(s)$ on the hyperboloid is a geodesic if and only if it satisfies:

$$\xi'' - \|\xi'\|_L^2 \xi = 0.$$

If $\|\xi'\|_L = 1$, then this equation corresponds to the parametrization by arc length. If we introduce the tangent vector $\eta = \xi'$, then we have the following equations:

$$\xi' = \eta, \qquad \eta' = -\|\eta\|_L^2 \xi,$$

with $\|\xi\|_L = -1$ and $\langle \xi, \eta \rangle_L = 0$, since tangent vectors to the hyperboloid are always perpendicular to the position vector of the point at which it is defined with respect to the Lorentzian inner product. These two equations represent the tangent bundle $T(F^d)$ of F^d, which we linearly idenfity with the cotangent bundle $T^*(F^d)$.

We now map the $T_1^*(\hat{F}^d)$ to $T^*(\mathbb{R}^d)$ by an extended hyperbolic stereographic projection. First we consider $T_1^*(\hat{F}^d)$ as a submanifold of $T^*(\mathbb{R}^{d+1})$, which we in turn identify with $\mathbb{R}^{d+1} \oplus \mathbb{R}^{d+1}$. In this embedding, $T_1^*(\hat{F}^d)$ corresponds to the pairs (ξ, η) such that $\|\xi\|_L = -1$, $\langle \xi, \eta \rangle_L = 0$ and $\|\eta\|_L = 1$. The canonical one-form $\theta_{\hat{F}^d}$ is the restriction of the canonical one-form on $T^*(\mathbb{R}^{d+1})$. We define the extended mapping by the following two equations:

$$\begin{aligned} x_k &= \frac{\xi_k}{1 - \xi_{d+1}}, \\ y_k &= (1 - \xi_{d+1})\eta_k + \xi_k \eta_{d+1}, \end{aligned}$$

for $k = 1, \ldots, d$. Its inverse is given by:

$$\begin{aligned} \xi_k &= \frac{2x_k}{1 - \|x\|^2}, \\ \xi_{d+1} &= \frac{\|x\|^2 + 1}{\|x\|^2 - 1}, \\ \eta_k &= \frac{1 - \|x\|^2}{2} y_k + \langle x, y \rangle x_k, \\ \eta_{d+1} &= -\langle x, y \rangle, \end{aligned}$$

for $k = 1, \ldots, d$.

These equations define a diffeomorphism. Let us check that the canonical one-forms $\theta_{\hat{F}^d}$ and $\theta_{\mathbb{R}^d}$ are mapped to each other. The canonical one-forms on $T^*\hat{F}^d$ and $T^*\mathbb{R}^d$ are given by $\theta_{\hat{F}^d} = \langle \eta, d\xi \rangle_L$ and $\theta_{\mathbb{R}^d} = \langle y, dx \rangle$ respectively.

If we substitute $dx_k = \frac{d\xi_k}{1-\xi_{d+1}} + \frac{d\xi_{d+1}}{(1-\xi_{d+1})^2}\xi_k$, we get

$$\begin{aligned}
\langle y, dx \rangle &= \sum_{k=1}^{d} y_k dx_k \\
&= \sum_{k=1}^{d} ((1-\xi_{d+1})\eta_k + \eta_{d+1}\xi_k) \left(\frac{d\xi_k}{1-\xi_{d+1}} + \frac{d\xi_{d+1}}{(1-\xi_{d+1})^2}\xi_k \right) \\
&= \sum_{k=1}^{d} \left(\eta_k d\xi_k + \frac{\eta_{d+1}}{1-\xi_{d+1}}\xi_k d\xi_k + \frac{\eta_k \xi_k d\xi_{d+1}}{1-\xi_{d+1}} + \eta_{d+1}\xi_k^2 \frac{d\xi_{d+1}}{(1-\xi_{d+1})^2} \right).
\end{aligned}$$

Using $0 = \frac{1}{2} d\|\xi\|_L^2 = \langle \xi, d\xi \rangle_L = \sum_{k=1}^{d} \xi_k d\xi_k - \xi_{d+1} d\xi_{d+1}$ in the second term and using the definition of the stereographic projection and the description of $T^*(F^d)$ as subspace of $\mathbb{R}^{d+1} \oplus \mathbb{R}^{d+1}$ gives us:

$$\begin{aligned}
&\sum_{k=1}^{d} \left(\eta_k d\xi_k + \frac{\eta_{d+1}}{1-\xi_{d+1}}\xi_k d\xi_k + \frac{\eta_k \xi_k d\xi_{d+1}}{1-\xi_{d+1}} + \eta_{d+1}\xi_k^2 \frac{d\xi_{d+1}}{(1-\xi_{d+1})^2} \right) \\
&= \sum_{k=1}^{d} \left(\eta_k d\xi_k + \frac{\eta_{d+1}}{1-\xi_{d+1}}\xi_{d+1} d\xi_{d+1} + \frac{\eta_{d+1}\xi_{d+1} d\xi_{d+1}}{1-\xi_{d+1}} + \eta_{d+1} d\xi_{d+1} \right) \\
&= \langle \eta, d\xi \rangle_L.
\end{aligned}$$

We can calculate that $\|\eta\|_L = \frac{(1-\|x\|^2)\|y\|}{2}$. In this way we get the following Hamiltonian:

$$F(x, y) = \Phi(\xi, \eta) = \frac{1}{2}\|\eta\|_L^2 = \frac{(1-\|x\|^2)^2\|y\|^2}{8},$$

which gives the following transformed Hamilton differential equations:

$$x' = F_y, \qquad y' = -F_x.$$

This set of equations follows from straightforward calculations. The geodesics such that $\|\eta\|_L = 1$ and $\Phi = \frac{1}{2}$ correspond to $F = \frac{1}{2}$. Now again comes the elegant trick. The differential equations form a system and the first partial derivatives of F are the only things which occur in the description. We can now replace F by $u(F) = \sqrt{2F} - 1$, because this defines a differentiable function at the point $F = \frac{1}{2}$ and $u'(\frac{1}{2}) = 1$. Now the gradients of both functions agree and thus we get for $G = u(F)$:

$$x' = G_y, \qquad y' = -G_x.$$

Note that the system on $F = \frac{1}{2}$ is now mapped to the system for which $G = 0$. If we change the variable s to:

$$t = \int \|y\| ds,$$

then $\dot{x} = \|y\|^{-1}x' = \|y\|^{-1}G_y$ and $\dot{y} = -\|y\|G_x$. If we define the following Hamiltonian:

$$H = \frac{1}{2}\|x\|^2 \pm \frac{1}{\|y\|} = \mp\|y\|^{-1}G + \frac{1}{2} = \mp\|y\|^{-1}(\sqrt{2F} - 1) + \frac{1}{2},$$

then we obtain the Hamilton equations $\dot{y} = H_x$ and $\dot{x} = -H_y$. So the Hamiltonian system (4.3) for $G = 0$ is mapped to this system with $H = \frac{1}{2}$. It is obvious that by the canonical transformation $p = x$ and $q = -y$, the system goes over into the Kepler problem. The trajectories of the geodesic flow on the hyperboloid away from the north pole parametrized by s are mapped to the trajectories of the Hamiltonian flow of $H = \frac{1}{2}\|x\|^2 \pm \frac{1}{\|y\|}$ away from $y \neq 0$ parametrized by t. The sign of the potential in H is determined by the sign of k. The trajectories for which $k = 1$ are mapped to geodesics on the positive sheet of the hyperboloid and the trajectories for which $k = -1$ to geodesics on the negative sheet. Note that this would interchange if we had chosen to perform a stereographic projection from the south pole.

A rescaling argument analogous to the one for negative energies. □

Again, by restoring the north pole, we obtain the regularization of the Kepler problem.

Remark 4.3.6. Geometrically, the north pole corresponds to the points at infinity in p-space, as can be seen from the geometry of the usual (non-extended) stereographic projection. In order to maintain a finite energy, it also corresponds to $q = 0$. The corresponding orbits are degenerated hyperbolas for which $k > 0$.

Corollary 4.3.7. For each $E > 0$, the energy regularized energy surface $\tilde{\Sigma}_E$ possesses $\mathrm{O}(d,1)$ symmetry. The infinitesimal symmetry is given by the Lorentz group $\mathfrak{o}(n,1)$. The group $\mathrm{O}(d,1)$ acts on the space $T_1^*(S^d)$ by matrix multiplication and takes geodesics (parametrized by arc length) into geodesics (parametrized by arc length).

If we would consider the group $\mathrm{O}(d,1)^\circ$, the connected component of the identity of $\mathrm{O}(d,1)$, then the Kepler orbits with $k = 1$ would be mapped to Kepler orbits with $k = 1$. Allowing all transformations of $\mathrm{O}(d,1)$ also interchanges geodesics with different k-signs.

In the next sections, we will describe another way of regularizing the Kepler problem. This method generalizes the whole negative (or the whole positive) phase space at once. We will prove that the corresponding regularization map is in fact a canonical deformation of the Moser map.

From now on, we restrict ourselves to the negative energy case, but remark that it can be formulated in the positive energy case as well. We also assume that $\mu = 1$ and $k = 1$.

4.4 The Delaunay Hamiltonian

Definition 4.4.1. Let T be the complement of the zero section of the cotangent bundle of the sphere, i.e.

$$T := \{(\xi, \eta) \in T^*(S^d) | \|\eta\| > 0\}.$$

The space T can be identified with a subspace of $\mathbb{R}^{d+1} \oplus \mathbb{R}^{d+1}$ as follows:

$$T \cong \{(x, y) \in \mathbb{R}^{d+1} \oplus \mathbb{R}^{d+1} \mid \|x\| = 1,\ \langle x, y\rangle = 0,\ y \neq 0\}.$$

As we have seen in the description of the relation between the Kepler orbits and the geodesic flow on the sphere, a reparametrization of the "time variable" occurs. In this section, we define a new Hamiltonian on T, whose Hamiltonian vector field is a time rescaling of the geodesic flow.

Remark 4.4.2. A moment map $\tilde{\mu} : T \to \mathfrak{so}(d+1)^*$ is given by $\tilde{\mu}(x, y) = x \wedge y$.

Definition 4.4.3. The **Delaunay Hamiltonian** $\tilde{H}$ on T is given by

$$\tilde{H}(\xi, \eta) = -\frac{1}{2}\frac{1}{\|\eta\|^2} = -\frac{1}{2}\frac{1}{\|\tilde{\mu}\|^2}.$$

Remark 4.4.4. It is obvious that $\tilde{H} = g \circ F$, where F is the geodesic Hamiltonian on the sphere and $g : \mathbb{R}_{>0} \to \mathbb{R}$, $z \mapsto -\frac{1}{4z}$.

Remark 4.4.5. The Hamiltonian vector field $X_{\tilde{H}}$ is a time rescaling of the geodesic vector field on T. In particular, its integral curves are geodesic curves on T.

The Delaunay Hamiltonian will turn out to be important for the following regularization procedure.

4.5 The Ligon-Schaaf map

We discuss another regularization of the Kepler problem. It leans heavily on integrals of motion and was described by Ligon and Schaaf [22]. Later Cushman and Duistermaat wrote down a more conceptual treatment of this regularization procedure [8], but they still rely on more calculations than necessary. The advantage of the method is that it regularizes the whole negative (or the whole positive) phase space of the Kepler problem at once, and it is a symplectomorphism.

We first give the Ligon-Schaaf map and briefly describe some properties formulated by Ligon and Schaaf. In addition, we will in detail describe how the Ligon-Schaaf regularization map arises naturally from the Moser method. This gives a geometrically well-formulated regularization procedure of the whole negative energy phase space of the Kepler problem.

We treat the regularization of the phase space P_- for negative energies here. Analogues for P_+ are true as well. The explicit Ligon-Schaaf map for the positive energy phase space can be found in [22].

For the Moser map Φ_M, as defined in section 4.3, the following holds.

Proposition 4.5.1. On the energy surface $\Sigma_{\frac{1}{2}}$, the **Moser map** $\Pi : T^*(\mathbb{R}^d) \to T_1^*(\hat{S}^d)$ is explicitly given by

$$\xi = \left(\|q\|p, \|q\|\|p\|^2 - 1\right), \qquad \eta = \left(\|q\|^{-1}q + \langle q, p\rangle p, -\langle q, p\rangle\right).$$

Φ_M is a canonical diffeomorphism.

Remark 4.5.2. The new claim of this proposition is the explicit form of the Moser map. It follows directly from the formulas of Section 4.3.

Definition 4.5.3. The **Ligon-Schaaf map** $\Phi_{LS} : P_- \to T$ is defined by

$$\Phi_{LS}(q,p) := \left((\cos\phi_{LS})\xi + (\sin\phi_{LS})\eta, (-2H)^{-\frac{1}{2}}\left((\sin\phi_{LS})\xi - (\cos\phi_{LS})\eta\right)\right),$$

where ξ and η are given by

$$\xi = \left((-2H)^{\frac{1}{2}}\|q\|p, \|q\|\|p\|^2 - 1\right), \qquad \eta = \left(\|q\|^{-1}q + \langle q, p\rangle p, -(-2H)^{-\frac{1}{2}}\langle q, p\rangle\right).$$

and

$$\phi_{LS} = -(-2H)^{\frac{1}{2}}\langle q, p\rangle \tag{4.5}$$

The following results are proved by Ligon and Schaaf.

Theorem 4.5.4. Φ_{LS} satisfies the following three properties:

1. Φ_{LS} is a diffeomorphism of P_- onto $T_- = \{(x,y) \in T \,|\, x \neq (0,\ldots,0,1)\}$;
2. Φ_{LS} is canonical;
3. if γ is an integral curve of the Kepler Hamiltonian vector field X_H in P_-, then $\Phi_{LS} \circ \gamma$ is a integral curve of the Delaunay Hamiltonian vector field $X_{\tilde{H}}$ in T;

Remark 4.5.5. The reason that the Ligon-Schaaf map regularizes the Kepler problem is that it defines a symplectic embedding of P_- onto T_- (in the slightly larger space T) whose Hamiltonian vector field is complete.

By comparison of the Moser map and the Ligon-Schaaf map, it might be the case that somehow the Moser map fits into the treatment by Ligon and Schaaf, because the components of the image of the Moser map are explicitly contained in the Ligon-Schaaf map, since $\nu = 1$ for $H = -\frac{1}{2}$. This motivates the definition of the Moser regularization fibration.

Definition 4.5.6. If we take ξ and η as defined in the Ligon-Schaaf map, then we define the **Moser regularization fibration** to be the map $\Pi_M : P_- \to T_1^*(\hat{S}^d)$ given by $\Pi_M(q,p) = (\xi, \eta)$.

Remark 4.5.7. Obviously, the restrictions of this map and the Moser map to the energy level $\Sigma_{-\frac{1}{2}}$ are the same.

Remark 4.5.8. If we change ϕ_{LS} in the Ligon-Schaaf map into the zero function, then we get the Moser regularization fibration fibration.

4.6 From Moser to Ligon-Schaaf

If we start with the Moser map, the Ligon-Schaaf map geometrically arises as the extension of it to P_-. The results of this section are also in [15]. In this article, also the details of the calculations regarding the symmetry group are given.

The relation between the geodesic flow given by F and the Delaunay flow is as follows.

Proposition 4.6.1. The geodesic flow of Hamiltonian $F = \frac{1}{2}\|\eta\|^2$ and the Delaunay flow of the Delaunay Hamiltonian $\tilde{H} = -\frac{1}{2\|\eta\|^2}$ are the same for $F = \frac{1}{2}$ and $\tilde{H} = -\frac{1}{2}$.

Proof. On $F = \frac{1}{2}$ we have:

$$d\tilde{H} = g'(F)dF = \frac{1}{4\frac{1}{2}^2}dF = dF.$$

Hence, the Hamiltonian vector fields match. □

The most important part of the argument, however, is the explicit relation between the arclength s and the real time t. A reparametrization of the time explicitly occurs in the Moser treatment. In the Ligon-Schaaf treatment it turns out to be implicitly done.

As was written before, the Kepler problem given by

$$\frac{dq}{dt} = p, \qquad \frac{dp}{dt} = -\|q\|^{-3}q$$

parametrized by t goes over by the Moser map in the (circular) geodesic motion given by

$$\frac{d\xi}{ds} = \eta, \qquad \frac{d\eta}{ds} = -\xi.$$

parametrized by s. The vectors ξ and η are orthonormal. If we define a complex structure on this plane by introducing the rotation by the angle $\frac{\pi}{2}$ in the counter-clockwise direction and call this i, then we get:

$$i\xi = \eta, \qquad i\eta = -\xi.$$

If we define

$$u = \exp(-i\langle q, p\rangle)\xi, \qquad v = (-2H)^{-\frac{1}{2}}\exp(-i\langle q, p\rangle)\eta,$$

then on $\Sigma_{-\frac{1}{2}}$ we obtain

$$\frac{du}{dt} = v, \qquad \frac{dv}{dt} = -u,$$

since

$$\frac{du}{dt} = -i\frac{d\langle q, p\rangle}{dt}u + \exp(-i\langle q, p\rangle)\frac{ds}{dt}\frac{d\xi}{ds} = (-p^2 + \frac{2}{q})v = v,$$

and a similar calculation for the second equation. This means that the circular motion parametrized by t is equivalent to the circular motion parametrized by s, which is in turn equivalent to the Kepler orbits parametrized by t. The multiplication by $\exp(-i\langle q,p\rangle)$ makes this relation explicit. Recall that $\eta_{d+1} = -\langle q,p\rangle$, so we can also write this factor in terms of the coordinates ξ and η.

We can use the actions defined on P_- and T_- to extend the Moser picture. Let ρ denote a parameter in $\mathbb{R}_{>0}$. Consider the rescaling function on P_- as defined earlier by

$$R_\rho(q,p,t,H) = (\rho^2 q, \rho^{-1}p, \rho^3 t, \rho^{-2}H).$$

We now also define a rescaling on T_- according to Ligon and Schaaf by

$$\tilde{R}_\rho(\xi,\eta,t,\tilde{H}) = (\xi, \rho\eta, \rho^3 t, \rho^{-2}\tilde{H})$$

Remark 4.6.2. Both scalings are well-defined.

Remark 4.6.3. Π_M is invariant under the scaling R_ρ, i.e. $\Pi_M(R_\rho(q,p)) = \Pi_M(q,p)$.

From direct calculations we obtain the following:

Proposition 4.6.4. The Ligon-Schaaf map intertwines both actions of $\mathbb{R}_+$, i.e.

$$\Phi_{LS} \circ R_\rho = \tilde{R}_\rho \circ \Phi_{LS}.$$

Theorem 4.6.5. The restriction of the Moser map Φ_M to the energy surface $\Sigma_{-\frac{1}{2}}$ extends to the symplectomorphism $\Phi_{LS} : P_- \to T_-$ by the scaling actions R and $\tilde{R}$.

Proof. If we perform the multiplication of $\exp(i\eta_{d+1})$ on the energy surface corresponding to $H = -\frac{1}{2}$, i.e.

$$(\xi,\eta) \mapsto \exp(i\eta_{d+1})(\xi,\eta) = (u,v)$$

the Moser map corresponds to the Ligon-Schaaf map on this energy surface, where now the curves of H and $\tilde{H}$ are now related by the same time t.

By the two actions of $\mathbb{R}_+$, which are intertwined by Φ_{LS}, this map extends to the whole P_- in a well-defined way. This gives the Ligon-Schaaf map as defined earlier.

This map is canonical. This follows from the canonicity of the Moser map and from the fact that $\Phi_{LS}^*\tilde{H} = H$, since Φ_{LS} is obtained from the Moser map by a canonical modification along the ruled surfaces with base the Kepler orbits in $\Sigma_{-\frac{1}{2}}$ and rulings the scale action. Indeed, on a surface S corresponding to a Kepler orbit, we have that $\omega|_S = dt \wedge dH|_S$ is mapped to $\tilde{\omega}|_{\Phi_{LS}(S)} = dt \wedge d\tilde{H}$. The scaling of $dt \wedge dH$ and $dt \wedge d\tilde{H}$ is consistent with the scaling of ω and $\tilde{\omega}$. □

This theorem gives the geometric relation between the regularization by Moser and the regularization by Ligon and Schaaf.

4.7 The symmetry group

Recall that the components of angular momentum and the Runge-Lenz vector are given by

$$L_{ij} = q_i p_j - q_j p_i,$$
$$K_i = (\|p\|^2 - \frac{1}{\|q\|})q_i - \langle q_i, p_i\rangle p_i$$

respectively.

Proposition 4.7.1. The following commutation relations hold for L_{ij}.

$$\{L_{ij}, L_{kl}\} = \delta_{jl}L_{ik} + \delta_{ik}L_{jl} - \delta_{jk}L_{il} - \delta_{il}L_{jk},$$

where $1 \leq i, j, k, l \leq d$.

This proposition is proved by straightforward calculations. From this proposition, it follows that the components L_{ij} for $1 \leq i, j \leq d$ generate the Lie algebra $\mathfrak{so}(d)$, which corresponds to the infinitesimal symmetry of the Kepler problem.

If we set

$$\frac{K_i}{\sqrt{-2H}} = L_{i(d+1)} = -L_{(d+1)i}$$

on P_-, then it turns out that the components L_{ij} for $1 \leq i, j \leq d+1$ generate the Lie algebra $\mathfrak{so}(d+1)$, which accounts for the hidden symmetry. In the literature, it is not well-motivated that the components of the Runge-Lenz vector come up as generators for the richer symmetry. The following theorem exhibits this symmetry of the Kepler problem by using the well-known symmetry of the complement T of the zero section of the cotangent bundle of the sphere and take the pull-back under the canonical Ligon-Schaaf map.

Theorem 4.7.2. If $M_{ij} := u_i v_j - v_i u_j$ are the components of angular momentum on $T \subset \mathbb{R}^{d+1} \oplus \mathbb{R}^{d+1}$, then

$$\Phi_{LS}^* M_{ij} = L_{ij}$$

for $1 \leq i, j \leq d+1$.

A proof of this theorem consists of straightforward calculations by writing out the expression $\Phi_{LS}^* M_{ij}$ at (q, p). This theorem proves that the Ligon-Schaaf map intertwines the infinitesimal actions of $\mathfrak{so}(d+1)$. We can integrate the Hamiltonian vector fields of L_{ij} to obtain an incomplete Hamiltonian action of $\mathrm{SO}(d+1)$. This action is regularized by the Ligon-Schaaf regularization. By definition, the Ligon-Schaaf map intertwines both actions of $\mathrm{SO}(d+1)$. From this, it follows that it also intertwines the moment maps.

Corollary 4.7.3. The Ligon-Schaaf map intertwines the two moment maps μ and $\tilde{\mu}$, i.e. $\mu(q, p) = \tilde{\mu}(\Phi_{LS}(q, p))$.

Remark 4.7.4. This property of the Ligon-Schaaf regularization map was proved by Ligon and Schaaf and was one of the key properties of this map in the article by Cushman and Duistermaat. They prove that this property and the three properties of Theorem 4.5.4 completely characterize the Ligon-Schaaf map.

Corollary 4.7.5. The commutation relations

$$\{L_{ij}, K_k\} = \delta_{ik}K_j - \delta_{jk}K_i,$$
$$\{K_i, K_j\} = -2HL_{ij}$$

follow from the fact that $\Phi_{LS}^* M_{ij} = L_{ij}$.

Note that the Runge-Lenz vector is indeed obtained as the integral of motion that accounts for the hidden symmetry.

Chapter 5

Quantization of the Kepler Hamiltonian

In this chapter, we look at possible quantizations of the Kepler Hamiltonian, which are operators that arise as the result of a quantization procedure applied to the classical Kepler Hamiltonian. Quantum mechanics has deterministic aspects if the Hamilton operator of a system is self-adjoint. The system is then said to be complete. We discuss in which way the classically incomplete Kepler problem gives rise to complete quantum Kepler problems by extending the naturally quantized Hamilton operator in a self-adjoint way. First we explain the idea of Schrödinger quantization, the framework in which the quantization of a Hamiltonian function fits. After some general theory about self-adjoint extensions, we then discuss the possible self-adjoint extensions of the quantum Kepler Hamiltonian.

5.1 Quantization procedures

In physics, the term **quantization** refers to any way of obtaining a quantum mechanical description of a physical system from its classical mechanical description. Even if we make this notion mathematically precise, there are several essentially different versions of it.

Definition 5.1.1. A **classical mechanical system** is a triple $(M, \{.,.\}, H)$ consisting of manifold M, the **phase space**, with a Poisson bracket $\{.,.\}$ on $C^\infty(M)$ and a smooth Hamiltonian function $H : M \to \mathbb{R}$.

Definition 5.1.2. A **quantum mechanical system** is a pair $(\mathcal{H}, \hat{H})$ consisting of a Hilbert space $\mathcal{H}$, playing the role of a "quantum phase space", with a self-adjoint operator $\hat{H}$, the **Hamilton operator**, defined on it.

Remark 5.1.3. On a Hilbert space, the **commutator bracket** $[A.B]$ of two operators A and B is formally defined as the operator $AB - BA$. The commutator bracket is a Lie bracket.

Remark 5.1.4. We distinguish in notation between the Hamiltonian function H and the Hamilton operator $\hat{H}$. We will, however, for simplicity call both objects the Hamiltonian.

Quantization relates classical and quantum mechanical systems. A **quantization procedure** assigns a quantum mechanical system $(\mathcal{H}, \hat{H})$ to each classical mechanical system $(M, \{.,.\}, H)$, i.e. $Q((M, \{.,.\}, H)) = (\mathcal{H}, \hat{H})$, in such a way that self-adjoint operators acting on $\mathcal{H}$ are assigned to functions in $C^\infty(M)$. There are many different versions of quantization, based on very different concepts. We will not go into this, since this goes beyond the scope of this thesis.

Remark 5.1.5. It turns out that it is not possible to find a quantization procedure that assigns a non-zero scalar operator to each non-zero constant function and such that the $\{.,.\}$ goes over into $\frac{i}{\hbar}[.,.]$ in a consistent way. This result is known as the Groenewold-Van Hove Theorem [13].

In the next section, we will describe Schrödinger quantization, since we defined the quantum Kepler problem as solving the Schrödinger equation of the Kepler problem.

5.2 Schrödinger quantization

The best well-known quantization procedure is **Schrödinger quantization**. Since we consider the Kepler problem, we restrict ourselves to classical systems with a configuration space $Q \subset \mathbb{R}^d$. The procedure of Schrödinger quantization maps the classical phase space, i.e. the cotangent bundle of the configuration space, to the Hilbert space $L^2(Q)$. Furthermore, the canonical coordinates are mapped to operators on this Hilbert space by

$$\begin{aligned} q_i &\mapsto q_i, \\ p_i &\mapsto -i\hbar\frac{\partial}{\partial q_i}. \end{aligned}$$

The image of the position coordinate q_i is the multiplication operator, given by multiplication by this coordinate. However, we do not distinguish in notation between the classical and the quantum case.

The Poisson brackets for q_i and p_j goes over in $\frac{i}{\hbar}[q_i, p_j]$ and the Hamiltonian function is mapped to the Hamilton operator. In this way, a particle with classical Hamiltonian $H = T + V$, where T is the kinetic energy and V the potential of the particle, is described quantum mechanically by its wave function $\Psi(x,t)$, which satisfies the **time-dependent Schrödinger equation**:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\psi(x,t), \tag{5.1}$$

where the Hamilton operator is obtained as the direct quantization of the classical Hamilton function, i.e.

$$\hat{H} = -\frac{\hbar^2}{2m}\Delta_{\mathbb{R}^d} + V,$$

where $\Delta_{\mathbb{R}^d}$ is considered as the restriction to the functions on Q that form a suitable domain, and V is a multiplication operator.

If the potential is time-independent, which is a physically quite weak assumption, and in particular it is the case for the Kepler problem, we can apply the method of separation of variables q and t. It is well-known that solving the time-dependent way then breaks down to solving the **time-independent Schrödinger equation**.

$$\hat{H}\psi = E\psi, \tag{5.2}$$

where $\Psi(x,t) = \psi(x)T(t)$. Solutions ψ of equation (5.2) are called **stationary states**.

5.3 Self-adjointness and quantum mechanics

In the time-independent Schrödinger equation, the Hamilton operator plays an essential role. If it is time-independent, we can define a time-evolution operator by:

$$U(t) = e^{-\frac{i\hat{H}t}{\hbar}}. \tag{5.3}$$

This gives us a solution of the time-dependent Schrödinger equation by

$$\Psi(x,t) = U(t)\Psi(x,0) =: U(t)\psi.$$

The operators $U(s)$ and $U(t)$ with $s,t \in \mathbb{R}$ satisfy

$$U(s)U(t) = U(s+t) = U(t+s) = U(t)U(s).$$

Moreover, $U(0) = 1$, the identity operator on $\mathcal{H}$.

We will now make the above precise. The formal properties of U are a motivation for the following definition.

Definition 5.3.1. A **unitary time-evolution** on a Hilbert space $\mathcal{H}$ is a unitary one-parameter group $\mathbb{R} \to \mathcal{U}(\mathcal{H}) \subset \mathcal{B}(\mathcal{H})$, $t \mapsto U(t)$ that is strongly continuous, i.e. $\|U(t)\psi - \psi\| \to 0$ for $t \to 0$ for all $\psi \in \mathcal{H}$.

Remark 5.3.2. Strong continuity is imposed as a consequence of the time-evolution of equation (5.1). The fact that the one-parameter group is unitary is motivated by equation (5.3).

We describe what conditions on the Hamiltonian give rise to unitary time-evolutions in the sense of Definition 5.3.1. It is obvious that if $\hat{H}$ is bounded and self-adjoint, then $U(t) = e^{-\frac{i\hat{H}t}{\hbar}}$ defines a unitary time-evolution. However, Hamilton operators are often unbounded and often not self-adjoint. The first turns out to be not very problematic, as explained by the following theorem. The latter often has to do with the domain of definition of the operator. If this is well-chosen, the operator may have a unique

self-adjoint extension. However, if the Hamiltonian is only symmetric, i.e. densely defined and $\langle \hat{H}x, y\rangle = \langle x, \hat{H}y\rangle$ for all $x, y \in \mathcal{H}$, then the operator may have infinitely many self-adjoint extensions. Different self-adjoint extensions can give rise to different time evolutions. The key result relating self-adjointness to unitary time-evolutions is Stone's Theorem [31, Section VIII.4].

Theorem 5.3.3. Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and let $U(t) := e^{itA}$ for $t \in \mathbb{R}$ be defined by the functional calculus. Then:

1. $\{U(t) \,|\, t \in \mathbb{R}\}$ is a strongly continuous unitary one-parameter group on $\mathcal{H}$;
2. if $\psi \in D(A)$, then $\lim_{t\to 0} \frac{1}{t}(U(t)\psi - \psi)$ exists and equals $iA\psi$;
3. if $\psi \in \mathcal{H}$ and $\lim_{t\to 0} \frac{1}{t}(U(t)\psi - \psi)$ exists, then $\psi \in D(A)$.

Conversely, if $\{U(t) \,|\, t \in \mathbb{R}\}$ is a strongly continuous unitary one-parameter group on $\mathcal{H}$, then there is a self-adjoint operator $(A, D(A))$ on $\mathcal{H}$ such that $U(t) = e^{itA}$ for all $t \in \mathbb{R}$.

5.4 Self-adjoint extensions

The goal of this section is to give the basic results of the theory of self-adjoint extensions of a closable symmetric[1] operator. Recall that for a closable symmetric operator A, we have $A \subset A^*$, i.e. A^* is an extension of A.

Definition 5.4.1. Let A be a closable symmetric operator with domain $\operatorname{Dom} A$. A **self-adjoint extension** A' of A is a self-adjoint operator such that $A \subset A' \subset A^*$. In particular, A' has the same action as A^* on a domain $\operatorname{Dom} A' \subset \operatorname{Dom} A^*$.

Remark 5.4.2. From this definition, it follows that in order to determine all self-adjoint extensions of an operator, one needs to find all possible domains of them, since the action is already known as the restriction of the action of its adjoint.

The results in this section are to be found in [9, 32, 37].

5.4.1 Spherical symmetry

A Schrödinger operator on (a, b) is the sum of minus the one-dimensional Laplacian and a potential function acting on a Hilbert space of the form $L^2(a, b)$ with $-\infty \leq a < b \leq \infty$. Such Schrödinger operators play an essential role in quantum mechanics, in particular if the quantum system studied is spherically symmetric. Indeed, after separation of variables, the radial part of the quantum Kepler Hamiltonian is of the desired form, as will be explained soon. In this case, whether or not the

[1] Recall that in the definition of a symmetric operator, it is implicitly assumed that it is densely defined.

resulting Schrödinger operator is self-adjoint is important for the study of possible time-evolutions of the quantum Kepler problem, since its self-adjointness is closely related to the self-adjointness of the Hamiltonian before separation of variables.

Separation of variables for spherical coordinates is used in the case of the Kepler problem. We assume that the reader is at least intuitively acquainted with this method and do not discuss it here. For more information and the application to the Schrödinger equation with a spherically symmetric potential, cf. [37, Chapter 18].

Recall that

$$L^2(\mathbb{R}^d) = L^2((0,\infty)\times S^{d-1}; r^{d-1}drd\Omega) = L^2((0,\infty); r^{d-1}dr)\hat{\otimes}L^2(S^{d-1}; d\Omega). \quad (5.4)$$

The Laplacian on the sphere has the set of spherical harmonics $Y_{l,j}$, where $l \in \mathbb{N}_0$ and $j = 1, \ldots, N(l,d) = \frac{(2l+d-2)(l+d-3)!}{l!(d-2)!}$ as a complete set of solutions. Define

$$X_{l,j} := \{f(r)Y_{l,j} \,|\, f \in L^2(0,\infty; r^{d-1}dr)\}$$

and

$$X^0_{l,j} := \{f(r)Y_{l,j} \,|\, f \in C_0^\infty(0,\infty)\}.$$

Then $X^0_{l,j}$ is dense in $X_{l,j}$. Because of equation (5.4) we have

$$L^2(\mathbb{R}^d) = \oplus_{l,j} X_{l,j}.$$

5.4.2 Deficiency indices

Definition 5.4.3. Let A be a symmetric operator on a Hilbert space $\mathcal{H}$. The **deficiency subspaces** $\mathcal{K}_+(A)$ and $\mathcal{K}_-(A)$ of A are defined by

$$\mathcal{K}_+(A) := \ker(A^* - i) = \mathrm{Ran}(A+i)^\perp,$$
$$\mathcal{K}_-(A) := \ker(A^* + i) = \mathrm{Ran}(A-i)^\perp.$$

Their dimensions $n_+(A) := \dim(\mathcal{K}_+)$ and $n_-(A) := \dim(\mathcal{K}_-)$ are called the **deficiency indices** of A.

From the deficiency indices, it is possible to conclude the family of self-adjoint extensions of A in two essentially different ways. First, we say what deficiency subspaces have to do with self-adjoint extensions.

Definition 5.4.4. A symmetric operator is called **essentially self-adjoint** if its closure is self-adjoint.

An essentially self-adjoint operator has a unique self-adjoint extension, namely its closure, which coincides with its adjoint.

Proposition 5.4.5. Let A be a symmetric operator. Then

1. A is essentially self-adjoint if and only if $n_+(A) = n_-(A) = 0$;

2. if $n_+(A) = n_-(A)$ then there is a one-to-one correspondence between self-adjoint extensions of A and unitary operators between $\mathcal{K}_+(A)$ and $\mathcal{K}_-(A)$, so if $n_+(A) = n_-(A) \geq 1$, then A has infinitely many self-adjoint extensions.

This proposition follows from [32, Theorem X.2]. We do not consider the case $n_+(A) \neq n_-(A)$, in which A has no self-adjoint extension at all.

5.4.3 Limit point-limit circle

We now investigate under which conditions on a potential V the corresponding Schrödinger operator is essentially self-adjoint. Conceptually, this is the case if the classical motion "stays away" from the points at infinity of the configuration space.

In what follows, let $V : (a, b) \to \mathbb{R}$ a locally square-integrable function with $-\infty \leq a < b \leq \infty$, i.e. $V \in L^2_{\text{loc}}(a, b)$.

Definition 5.4.6. The **minimal Schrödinger operator** H with potential V on the interval (a, b) is the operator H with domain $\operatorname{Dom} H := C_0^\infty(a, b)$ and action

$$H = -\frac{d^2}{dx^2} + V(x).$$

Recall that a function $f : (a, b) \to \mathbb{C}$ is called absolutely continuous if for every $\varepsilon > 0$ there exists a $\delta > 0$ such that if $(a_1, b_1), \ldots, (a_n, b_n)$ is a collection of finitely many pairwise disjoint intervals in (a, b) with

$$\sum_{i=1}^{n} (b_i - a_i) < \delta$$

then

$$\sum_{i=1}^{n} |f(b_i) - f(a_i)| < \varepsilon.$$

Proposition 5.4.7. The domain $\operatorname{Dom} H^*$ of the adjoint of the minimal Schrödinger operator H of the previous definition is given by

$$\operatorname{Dom} H^* = \{\psi \in L^2(a, b) \,|\, \psi, \psi' \in \mathrm{AC}(a, b), H^*\psi \in L^2(a, b)\},$$

where $\mathrm{AC}(a, b)$ denotes the set of absolutely continuous functions on (a, b). The operator H^* acts by the same action of H extended to the absolutely continuous functions. This domain is dense in $L^2(a, b)$.

Remark 5.4.8. Recall that an operator A is closable if and only if A^* is densely defined. It follows that minimal Schrödinger operators are closable.

Definition 5.4.9. A function $f : (a, b) \to \mathbb{C}$ is called square-integrable at a if there exists a $c \in (a, b)$ such that $f \in L^2(a, c)$. A function $f : (a, b) \to \mathbb{C}$ is called square-integrable at b if there exists a $c \in (a, b)$ such that $f \in L^2(c, b)$.

Definition 5.4.10. The potential V is said to be in the **limit circle** case at a (at b) if for some —and therefore all [37, Theorem 13.17]— $\lambda \in \mathbb{C}$ all solutions ψ of the Schrödinger equation $H\psi = \lambda\psi$, where H is the minimal Schrödinger operator from Definition 5.4.6, are square-integrable at a (at b). If V is not at the limit circle case at a (at b), then it is said to be in the **limit point** case at a (at b).

Theorem 5.4.11. The operator H is essentially self-adjoint if and only if the corresponding V is in the limit point case at both a and b.

A proof of this theorem is found at [9, Theorem 7.2.13]. If a symmetric operator is not essentially self-adjoint, it is possible that is has infinitely many self-adjoint extensions. Below, we describe two ways to determine them.

5.4.4 Von Neumann theory

The following theorem by von Neumann characterizes all self-adjoint extensions in terms of the closure. It follows from [9, Section 2.5].

Theorem 5.4.12. Let A be a closable symmetric operator on a Hilbert space $\mathcal{H}$. Then A' is a self-adjoint extension if A' has the same action as A^* and domain

$$\operatorname{Dom} A' = \operatorname{Dom} A_U := \{\psi + \psi_- - U\psi_- \,|\, \psi \in \operatorname{Dom} \overline{A},\, \psi_- \in \mathcal{K}_-(A)\},$$

where $U : \mathcal{K}_-(A) \to \mathcal{K}_+(A)$ is a unitary map between the deficiency spaces.

5.4.5 Boundary forms

Boundary forms are sesquilinear maps from the domain of an adjoint to $\mathbb{C}$, which classify the self-adjoint extensions of a symmetric operator explicitly by means of the unitary operators between the deficiency subspaces.

Definition 5.4.13. Let A be a symmetric operator. Define the **boundary form** corresponding to A as the sesquilinear map $\Gamma := \Gamma_{A^*} : \operatorname{Dom} A^* \times \operatorname{Dom} A^* \to \mathbb{C}$ given by

$$\Gamma(f, g) := \langle A^* f, g\rangle - \langle f, A^* g\rangle$$

for $f, g \in \operatorname{Dom} A^*$.

The following result, a proof of which is found at [9, Proposition 7.1.8], classifies the self-adjoint extensions explicitly.

Proposition 5.4.14. Let A be a symmetric operator with equal deficiency indices. Then each unitary operator $U : \mathcal{K}_-(A) \to \mathcal{K}_+(A)$ gives rise to a self-adjoint extension with domain

$$\operatorname{Dom} A_U = \{f \in \operatorname{Dom} A^* \,|\, \Gamma(f, g - Ug) = 0\, \forall g \in \mathcal{K}_-(A)\}$$

and action $A_U f = A^* f$.

There are convenient ways of finding the unitaries U.

Definition 5.4.15. Let A be a symmetric operator such that $n_-(A) = n_+(A)$. We define a **boundary triple** $(\mathcal{L}, \rho_1, \rho_2)$ for A as a Hilbert space $\mathcal{L}$ and two linear maps $\rho_1, \rho_2 : \operatorname{Dom} A^* \to \mathcal{L}$ with dense ranges such that

$$a\Gamma_A^*(f,g) = \langle \rho_1(f), \rho_1(g)\rangle - \langle \rho_2(f), \rho_2(g)\rangle$$

for all $f, g \in \operatorname{Dom} A^*$ and some constant $0 \neq a \in \mathbb{C}$.

Proposition 5.4.16. Let A be a symmetric operator such that $n_-(A) = n_+(A)$. If $(\mathcal{L}, \rho_1, \rho_2)$ is a boundary triple for A, then the self-adjoint extension A_U of A corresponding to the unitary map unitary map $U : \mathcal{L} \to \mathcal{L}$ is the operator with domain

$$\operatorname{Dom} A_U = \{f \in \operatorname{Dom} A^* \,|\, \rho_2(f) = U\rho_1(f)\}$$

and action $A_U f = A^* f$.

A proof of this proposition is found at [9, Theorem 7.1.13].

5.5 The quantum Kepler Hamiltonian

We now return to the problem of quantizing the quantum Kepler Hamiltonian. For our purposes in this chapter, this part of the Schrödinger quantization procedure is the most important.

The results in this chapter are taken from [9, 32, 36, 37]. There, one can also find details and proofs. It is possible to say much more.

Remark 5.5.1. In this chapter, we leave our notation in coordinates q and p and use r and Ω instead to emphasize that we are working in spherical coordinates.

The d-dimensional quantum Kepler Hamiltonian is initially defined as the operator

$$\hat{H} : \mathcal{D} \to L^2(\mathbb{R}^d)$$

given by

$$\hat{H} = -\Delta_{\mathbb{R}^d} - \frac{k}{r},$$

where $r = \|(x_1, \ldots, x_d)\|$ and

$$\mathcal{D} = C_0^\infty(\mathbb{R}^d \setminus \{0\}).$$

Note that this operator is not self-adjoint on this domain. Using separation of variables, the Laplacian on $\mathbb{R}^d$ is given by

$$\Delta_{\mathbb{R}^d} = \frac{\partial^2}{\partial r^2} + \frac{d-1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Delta_{S^d},$$

where Δ_{S^d} is the Laplacian on the d-sphere.

The quantum Kepler Problem is to determine the eigenvalues and eigenfunctions of the Schrödinger equation

$$\hat{H}\psi = E\psi.$$

Physically, this problem corresponds to determining the energy levels and corresponding electron disctributions of the hydrogen atom.

Remark 5.5.2. The physical version of the quantum Kepler Hamiltonian contains some constants, such as $\hbar$ and μ. For our purposes, the values of these constants do not matter, as long as they are positive. Therefore, it is harmless to set $\hbar = 1$ and $\mu = \frac{1}{2}$, as we did.

5.6 Self-adjoint extensions of the Kepler Hamiltonian

In this section, we discuss the self-adjoint extensions of the quantum Kepler Hamiltonian. To this end, we distuinguish between different dimensions. It is expected that in higher dimensions, there is "less to choose" than in the lower dimensions, because of the topological nature of the singularity at 0.

The results in this section are explicitly given for the Kepler Hamiltonian. Many can be generalized to other potentials, but we do not make the proofs lengthier to that purpose, as this text is about the Kepler problem. For the general results, cf. [32, 37].

First, we consider the cases $d \geq 4$ and $d = 3$, then the case $d = 2$, and finally $d = 1$. For both the case $d \geq 4$ and the case $d = 3$, which we need to treat separately later, we consider the operator $\hat{H}$ on domain $\mathcal{D} := C_0^\infty(\mathbb{R}^d \setminus \{0\})$ with $d \geq 3$. Recall our definition of $X_{l,j}$ and $X_{l,j}^0$:

$$X_{l,j} := \{f(r)Y_{l,j} \mid f \in L^2(0,\infty; r^{d-1}dr)\} X_{l,j}^0 := \{f(r)Y_{l,j} \mid f \in C_0^\infty(0,\infty)\}.$$

Proposition 5.6.1. The operator $\hat{H}$ maps $X_{l,j}^0$ to $X_{l,j}$

Proof.

$$\begin{aligned}\hat{H}(f(r)Y_{l,j}(\theta)) &= \left(-\frac{d^2f}{dr^2} - \frac{d-1}{r}\frac{df}{dr} - \frac{kf(r)}{r}\right) Y_{l,j}(\theta) - \frac{f(r)}{r^2}\Delta_{S^{d-1}}Y_{l,j}(\theta) \\ &= \left(-\frac{d^2f}{dr^2} - \frac{d-1}{r}\frac{df}{dr} - \frac{kf(r)}{r} + \frac{l(l+d-2)}{r^2}f(r)\right) Y_{l,j},\end{aligned}$$

which is an element of $X_{l,j}$. □

From this, it follows that the restriction of $\hat{H}$ to $X_{l,j}^0$ is unitary equivalent to

$$\hat{H}_l' := -\frac{d^2}{dr^2} - \frac{d-1}{r}\frac{d}{dr} - \frac{k}{r} + \frac{l(l+d-2)}{r^2}$$

with domain $C_0^\infty(0,\infty) \subset L^2(0,\infty; r^{d-1}dr)$, since $\hat{H}$ only depends on l and not on j on the domain $X_{l,j}^0$. It follows that $\hat{H}_l'$ is symmetric on this domain.

Proposition 5.6.2. If we define $\hat{H}_l$ by

$$\hat{H}_l := U\hat{H}'_l U^{-1},$$

where $U : L^2(0,\infty; r^{d-1}dr) \to L^2(0,\infty)$ is the unitary operator given by $(Uf)(r) = r^{\frac{d-1}{2}} f(r)$, then $\hat{H}_l$ acts on $C_0^\infty(0,\infty) \subset L^2(0,\infty)$ by

$$\hat{H}_l = -\frac{d^2}{dr^2} + \left(l(l+d-2) + \frac{1}{4}(d-1)(d-3)\right)\frac{1}{r^2} - \frac{k}{r}.$$

In particular, $\hat{H}_l$ and $\hat{H}'_l$ are unitary equivalent.

Proof. It is obvious, U being a unitary operator, that $\hat{H}_l$ and $\hat{H}'_l$ are unitary equivalent. The action of $\hat{H}_l$ is obtained by writing out $U\hat{H}'_l U^{-1}$.

$$\begin{aligned}
(\hat{H}_l f)(r) &= (U\hat{H}'_l U^{-1} f)(r) \\
&= (U\hat{H}'_l) r^{-\frac{d-1}{2}} f(r) \\
&= U(-\frac{(d-1)(d+1)}{4} r^{-\frac{d+3}{2}} f(r) + (d-1) r^{-\frac{d+1}{2}} \frac{df(r)}{dr} - r^{-\frac{d-1}{2}} \frac{d^2 f(r)}{dr^2} \\
&+ \frac{(d-1)^2}{2r} r^{-\frac{d+1}{2}} f(r) - \frac{d-1}{r} r^{-\frac{d-1}{2}} \frac{df(r)}{dr} + \frac{l(l+d-2)}{r^2} r^{-\frac{d-1}{2}} f(r) \\
&- \frac{k}{r} r^{-\frac{d-1}{2}} f(r)) \\
&= -\frac{(d-1)(d+1)}{4r^2} f(r) + \frac{(d-1)}{r}\frac{df(r)}{dr} - \frac{d^2 f(r)}{dr^2} \\
&+ \frac{(d-1)^2}{2r^2} f(r) - \frac{d-1}{r}\frac{df(r)}{dr} + \frac{l(l+d-2)}{r^2} f(r) - \frac{k}{r} f(r),
\end{aligned}$$

□

Write $W(r) := \left(l(l+d-2) + \frac{1}{4}(d-1)(d-3)\right)\frac{1}{r^2} - \frac{k}{r}$ and consider it as an effective potential.

5.6.1 Dimension $d \geq 4$

For the treatment of this case, we follow [37, Section 18.3].

Lemma 5.6.3. For $d \geq 4$, the potential W is in the limit point case at 0.

Proof. For $d \geq 5$ and $l \in \mathbb{N}_0$, as well as for $d = 4$ and $l \geq 1$, we have $W(r) \geq \frac{3}{4} r^{-2}$ for small r. Hence [32, Theorem X.10] applies.

For the case $d = 4$ and $l = 0$, the effective potential takes the form $W(r) = \frac{3}{4} r^{-2} + V(r)$. We use the fact that V has $-\Delta$-bound 0 [37, Theorem 17.2]. From this, it follows that V has also $-\Delta + \frac{3}{4} r^{-2}$-bound 0. Because $\frac{3}{4} r^{-2}$ is in the limit point case at 0, also W is in the limit point case at 0, which follows from [36, Theorem 10.4]. □

Lemma 5.6.4. For $d \geq 3$, the potential W is in the limit point case at ∞.

Proof. This result follows from [32, Theorem X.8] by choosing a large enough constant function for $M(r)$. This works, because W has a minimum on $(0, \infty)$. □

From these two lemmas, it follows that $\hat{H}_l$ is essentially self-adjoint for all $l \in \mathbb{N}_0$. Let T_l denote the (unique) self-adjoint extension of $\hat{H}_l$ for $l \in \mathbb{N}_0$. Recall the following proposition about the sum of self-adjoint operators [37, Theorem 18.2].

Proposition 5.6.5. If A_i with domain $\mathrm{Dom}(A_i)$ denotes a self-adjoint operator on the Hilbert space $\hat{\mathcal{H}}_i$ for each $i \in \mathbb{I}$, then the orthogonal sum $A = \oplus_{i \in \mathbb{I}} A_i$ is a self-adjoint operator on $\oplus_{i \in \mathbb{I}} \hat{\mathcal{H}}_i$.

From Lemma 5.6.3 and Lemma 5.6.4, the following result is immediate.

Theorem 5.6.6. The operator $\oplus_{l \in \mathbb{N}_0, j=1,\ldots,N(l,d)} T_l$ is a self-adjoint operator.

Remark 5.6.7. This self-adjoint extension is unitary equivalent to the (unique) self-adjoint extension of $\hat{H}$ with domain $C_0^\infty(\mathbb{R}^d)$.

Corollary 5.6.8. The Hamilton operator $\hat{H}$ admits a unique unitary time-evolution. So the quantum Kepler problem for $d \geq 4$ is complete.

Remark 5.6.9. Note that the Kepler problem for $d \geq 4$ is an example of a problem which is complete in the quantum description, but incomplete in the classical description.

5.6.2 Dimension $d = 3$

For the treatment of the three-dimensional case, we use the same methods as for the higher-dimensional case, but the result is different. We expose the material in the same way as before. The technical details are due to [10].

Define $\hat{H}_l'$ and $\hat{H}_l$ in the same way as above. Their form is the same. Moreover, we can substitute $d = 3$, which yields

$$\hat{H}_l := -\frac{d^2}{dr^2} + \frac{l(l+1)}{r^2} - \frac{k}{r}.$$

The potential $W(r) = \frac{l(l+1)}{r^2} - \frac{k}{r}$ is in the limit point case at ∞, which was proved in Lemma 5.6.4. By an analogous argument as in Lemma 5.6.3 to prove that $W(r)$ is in the limit point case at 0 for $d \geq 4$ and $l \geq 1$, we conclude that for $d = 3$ and $l \geq 1$ is in the limit point case, since then also $W(r) \geq \frac{3}{4} r^{-2}$ for small r.

Lemma 5.6.10. For $d = 3$ and $l = 0$, the potential $W(r)$ is in the limit circle case.

Proof. Because for $l = 0$ we have $W(r) = \frac{k}{r} \leq \frac{C}{r^2}$ for all $C > 0$ and small enough r, it follows that $W(r)$ is in the limit circle case at 0 [32, Theorem X.10] . □

Denote by $\hat{H}_l^*$ the (unique) self-adjoint extension of $\hat{H}_l$ by for $l \geq 1$. Recall ([9, Proposition 2.3.20]) that the domain of $\hat{H}_l^*$ (and its adjoint) is given by

$$D(\hat{H}_l^*) = \{f \in L^2(0,\infty) \,|\, f, f' \in \mathrm{AC}(0,\infty), \hat{H}_l^* f \in L^2(0,\infty)\}, \tag{5.5}$$

where $\hat{H}_l^*$ has the same action as $\hat{H}_l$.

By [9, Theorem 2.1.24], the adjoint T^* of an Hermitean operator T is an extension of all self-adjoint extensions of T. So in the case $l = 0$, we look for extensions $\tilde{\hat{H}}_0$ of $\hat{H}_0$ with domain D such that $\mathrm{Dom}\,\hat{H}_0 \subset D \subset \mathrm{Dom}\,\hat{H}_0^*$ and the same —but restricted— action as $\hat{H}_0^*$.

In order to determine these self-adjoint extensions explicitly, we use the following lemma [10, Lemma 1].

Lemma 5.6.11. For $g \in \mathrm{Dom}\,\hat{H}_0^*$, the lateral limits

$$g(0^+) := \lim_{r\to 0^+} g(r),$$
$$\tilde{g}(0^+) := \lim_{r\to 0^+} (g'(r) + g(r)\log(r))$$

exist and are finite.

The **boundary form** corresponding to $\hat{H}_0$ is defined as

$$\Gamma(f,g) := \langle \hat{H}_0^* f, g\rangle - \langle f, \hat{H}_0^* g\rangle$$

for $f, g \in \mathrm{Dom}\,\hat{H}_0^*$. Using Lemma 5.6.11 and integration by parts, it follows [10] that

$$\Gamma(f,g) = -\left(f(0^+)\overline{\tilde{g}(0^+)} - \tilde{f}(0^+)\overline{g(0^+)}\right).$$

The results of Subsection 5.4.5 give us a way to explicitly determine the self-adjoint extensions of $\hat{H}_0$. For $f \in \mathrm{Dom}\,\hat{H}_0^*$, define

$$\rho_\pm(f) := f(0^+) \pm i\tilde{f}(0^+)$$

The ranges images of $\rho_\pm$ are dense in $\mathbb{C}$. It follows that

$$\langle \rho_+(f), \rho_+(g)\rangle_{X_+} - \langle \rho_-(f), \rho_-(g)\rangle_{X_-} = 2i\Gamma(f,g), \tag{5.6}$$

where $\langle ., .\rangle_{X_\pm}$ denotes the standard inner product on $X_\pm$ and $f, g \in \mathrm{Dom}\,\hat{H}_0^*$.

By [37, Theorem 13.19], $\hat{H}_0$ has deficiency indices equal to 1. By Proposition 5.4.16, finding the domains D for which equation (5.6) holds, comes down to determining, for each unitary operator $U : \mathcal{L} \to \mathcal{L}$, the elements f of $\mathrm{Dom}\,\hat{H}_0^*$ such that $U\rho_+(f) = \rho_-(f)$. Explicitly, the unitary mappings between one-dimensional Hilbert spaces are given by $\{U_\theta := e^{i\theta} \,|\, \theta \in [0, 2\pi)\}$. These all give rise to an extension with domain

$$\mathrm{Dom}\,\hat{H}_{0,\theta} = \{f \in \mathrm{Dom}\,\hat{H}_0^* \,|\, (1 - e^{i\theta})f(0^+) = i(1 + e^{i\theta})\tilde{f}(0^+)\}.$$

For $\theta \neq 0$, this is equivalent to

$$f(0^+) = \lambda\tilde{f}(0^+), \qquad \lambda = i\frac{1 + e^{i\theta}}{1 - e^{i\theta}} \in \mathbb{R}.$$

For $\theta = 0$, we set $\lambda = \infty$. The following result follows.

Proposition 5.6.12. The self-adjoint extensions $\hat{H}_0^\lambda$ with $\lambda \in \mathbb{R} \cup \{\infty\}$ have domain

$$\operatorname{Dom} \hat{H}_0^\lambda = \{f \in \operatorname{Dom} \hat{H}_0^* \mid f(0^+) = \lambda \tilde{f}(0^+)\}$$

and action

$$\hat{H}_0^\lambda f = \hat{H}_0^* f.$$

The following theorem now holds.

Theorem 5.6.13. The self-adjoint extensions of $(\hat{H}, C_0^\infty(\mathbb{R}^3 \setminus \{0\}))$ are

$$\hat{H}_\lambda = (U^{-1} \hat{H}_0^\lambda U \otimes I_0) \oplus \bigoplus_{l=1}^{\infty} (U^{-1} \hat{H}_l^* U \otimes I_l), \qquad \lambda \in \mathbb{R} \cup \{\infty\},$$

where each summand acts on its specified domain and I_l ($l \geq 0$) denotes the identity operator on $X_{l,j}$.

5.6.3 Dimension $d = 2$

For the treatment of the 2-dimensional quantum Kepler problem, we follow [10]. Hereto, consider the operator $\hat{H}$ on domain $C_0^\infty(\mathbb{R}^2 \setminus \{0\})$. We only sketch the arguments here and do not treat the explicit properties of the special functions involved.

In two dimensions, the Laplacian has the following form:

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}.$$

By the theory of spherical harmonics, the eigenfunctions of the Laplacian are given by

$$\frac{d^2}{d\theta^2} Y_l(\theta) = -l^2 Y_l(\theta).$$

It follows that an orthogonal base of eigenfunctions is given by

$$\{e^{il\theta} \mid l \in \mathbb{Z}\}.$$

Remark 5.6.14. The eigenspace corresponding to the eigenvalue $-l^2$ for $l \neq 0$ is two-dimensional and the eigenspace corresponding to the eigenvalue 0 is one-dimensional, which is in agreement with the numbers $N(l, 2)$, which give the multiplicity of the eigenspaces.

Let now X_l denote the space $X_l := \{f(r)Y_l \mid f \in L^2(0, \infty; rdr)\}$ and likewise $X_l^0 := \{f(r)Y_l \mid f \in C_0^\infty(0, \infty)\}$. Obviously $\hat{H}$ maps X_l^0 to X_l and just as in the higher-dimensional case, the restriction $\hat{H}_l$ of $\hat{H}$ to X_l is unitary equivalent to the operator

$$\hat{H}_l' = -\frac{d^2}{dr^2} - \frac{1}{r}\frac{d}{dr} - \frac{k}{r} + \frac{l^2}{r^2},$$

with domain $C_0^\infty(0,\infty) \subset L^2(0,\infty; rdr)$. The unitary transformation $(Uf)(r) = r^{\frac{1}{2}} f(r)$ shows that $\hat{H}_l$ is unitary equivalent to

$$\hat{H}_l := U\hat{H}_l' U^{-1} = -\frac{d^2}{dr^2} - \frac{k}{r} + \frac{l^2 - \frac{1}{4}}{r^2},$$

with domain $C_0^\infty(0,\infty) \subset L^2(0,\infty)$.

Remark 5.6.15. Let $l \neq 0$. The fact that $W(r) = \frac{l^2-\frac{1}{4}}{r^2} - \frac{k}{r}$ is in the limit point case at ∞ again follows from [32, Theorem X.8].

We now prove that $W(r)$ is in the limit point case at 0 for $l \neq 0$ and in the limit circle case at 0 for $l = 0$. To this end, we look at the eigenfunctions of $\hat{H}_l^* \psi = \lambda\psi$ for $\lambda = i$. We obtain the following equation:

$$-\psi'' + \left((l^2 - \frac{1}{4}) \frac{1}{r^2} - \frac{k}{r} - i \right) \psi = 0.$$

Changing variables to $y = \sqrt{-4i}r$, this equation takes the form

$$\psi'' + \left((\frac{1}{4} - l^2) \frac{1}{y^2} + \frac{k}{\sqrt{-4i}y} - \frac{1}{4} \right) \psi = 0, \tag{5.7}$$

and we prove that this equation has solutions that are not square-integrable at 0, which implies that W is limit point at 0.

Equation (5.7) is solved by the Whittaker functions [38]. For $l = 0$, these functions are square-integrable at 0; for $l \neq 0$, some Whittaker functions are not square-integrable at 0. So W is in the limit circle case at 0 for $l = 0$ and is in the limit point case for $l \neq 0$.

From these facts, the following result follows.

Proposition 5.6.16. The operator $\hat{H}_l$ is essentially self-adjoint for $l \neq 0$. The operator $\hat{H}_0$ has deficiency indices equal to 1.

For $l \neq 0$, let T_l denote the (unique) self-adjoint extension of $\hat{H}_l$. The Whittaker function $M_-(y) := M_{(-4i)^{-\frac{1}{2}},0}(y)$ spans the deficiency subspace $\mathcal{K}_-$, since this is a square-integrable solution at 0. The deficiency subspace $\mathcal{K}_+$ is spanned by the function $M_+(y) := \overline{M(y)}$. In this case, from the von Neumann theory of self-adjoint extensions (cf. Subsection 5.4.4), the following result follows.

Proposition 5.6.17. The self-adjoint extensions $\hat{H}_0^\theta$ of $\hat{H}_0$ are the operators with domain

$$\operatorname{Dom} \hat{H}_{0,\theta} = \{\psi + c(\phi_+ - e^{i\theta}\phi_-) \,|\, \psi \in \operatorname{Dom} \overline{\hat{H}_0}, c \in \mathbb{C}\},$$

where $\phi_\pm$ defined as above, and action $\hat{H}_{0,\theta}\psi = \hat{H}_0^*\psi$.

Proof. The unitary operators from $\mathcal{K}_-(\hat{H}_0)$ to $\mathcal{K}_+(\hat{H}_0)$ are again multiplications by $e^{i\theta}$ and the complex conjugation. □

Theorem 5.6.18. The self-adjoint extensions $\hat{H}_\theta$ of $\hat{H}$ on $C_0^\infty(\mathbb{R}^2 \setminus \{0\})$ are given by

$$\hat{H}_\theta = (U^{-1}\hat{H}_{0,\theta}U) \oplus \bigoplus_{l\in\mathbb{Z}\setminus\{0\}} (U^{-1}T_l U),$$

where each summand acts on its specified domain.

5.6.4 Dimension $d = 1$

The one-dimensional case is the most subtle, since the natural domain of definition of the Hamiltonian is not even connected. There is a lot to say about this [9, 10]. We only give a more sketchy overview than for the cases of other dimensions. In [10], some physical considerations are discussed as well.

Consider the one-dimensional quantum Kepler Hamiltonian with natural domain $C_0^\infty(\mathbb{R} \setminus \{0\})$. This domain is not connected. Therefore, the one-dimensional case needs to be considered carefully, since we need to deal with the behaviour of the solutions near zero from two sides that do not have to do anything with another at first.

Let us write $C_0^\infty(\mathbb{R} \setminus \{0\}) = C_0^\infty(-\infty, 0) \oplus C_0^\infty(0, \infty)$ and define $\hat{H}_1 := \hat{H}|_{C_0^\infty(-\infty,0)}$ and $\hat{H}_2 := \hat{H}_{C_0^\infty(0,\infty)}$. Thus, $\hat{H} = \hat{H}_1 \oplus \hat{H}_2$. The domain of the adjoint of $\hat{H}_1$ is given by

$$\operatorname{Dom} \hat{H}_1^* = \{f \in L^2(0,\infty) \mid f, f' \in \mathrm{AC}(0,\infty), \hat{H}_+^* f \in L^2(0,\infty)\},$$

and a similar expression holds for $\hat{H}_2$. It follows that

$$\operatorname{Dom} \hat{H}^* = \{f \in L^2(\mathbb{R}) \mid f, f' \in \mathrm{AC}(\mathbb{R} \setminus \{0\}), \hat{H}^* f \in L^2(\mathbb{R})\}.$$

The method of finding self-adjoint extension that we applied in higher dimensions can also be used for the one-dimensional problem, but we need to distinguish more cases. First, we state an analogue of Lemma 5.6.11.

Lemma 5.6.19. 5.6.11 For $g \in \operatorname{Dom} \hat{H}^*$, the lateral limits

$$g(0^\pm) := \lim_{h\to 0^\pm} g(x),$$
$$\tilde{g}(0^\pm) := \lim_{h\to 0^\pm} (g'(x) \pm g(x)\ln(|x|))$$

exist and are finite.

A proof of this lemma can be found in [9, Lemma 7.4.3]. In [25], the following result is proved.

Proposition 5.6.20. For the deficiency indices, the following holds:

$$n_+(\hat{H}_\pm) = n_-(\hat{H}_\pm) = 1,$$
$$n_+(\hat{H}) = n_-(\hat{H}) = 2.$$

It follows that the boundary form takes the form

$$\Gamma(f,g) = \overline{f(0^+)}\tilde{g}(0^+) - \overline{\tilde{f}(0^+)}g(0^+) + \overline{\tilde{f}(0^-)}g(0^-) - \overline{f(0^-)}\tilde{g}(0^-).$$

For $f \in \operatorname{Dom} \hat{H}^*$, define $\rho_1, \rho_2 : \operatorname{Dom} \hat{H}^* \mathbb{C}^2$ by

$$\rho_1(f) := \begin{pmatrix} \tilde{f}(0^+) + if(0^+) \\ \tilde{f}(0^-) - if(0^-) \end{pmatrix},$$
$$\rho_2(f) := \begin{pmatrix} \tilde{f}(0^+) - if(0^+) \\ \tilde{f}(0^-) + if(0^-) \end{pmatrix}.$$

It follows that

$$\langle \rho_1(f), \rho_1(g) \rangle_{\mathbb{C}^2} - \langle \rho_2(f), \rho_2(g) \rangle_{\mathbb{C}^2} = -2i\Gamma(f,g),$$

where $f, g \in \operatorname{Dom} \hat{H}_0^*$. We proceed in the same way as in for the previous cases. Each unitary matrix $U \in \operatorname{Mat}_2(\mathbb{C})$ gives rise to a self-adjoint extension $\hat{H}_U$ with domain

$$\operatorname{Dom} \hat{H}_U = \{ f \in \operatorname{Dom} \hat{H}^* \mid \rho_2(f) = U\rho_1(f) \}$$

and the same action as $\hat{H}^*$.

5.7 Completeness of the quantum Kepler problem

Definition 5.7.1. A quantum system on a Hilbert space $\hat{\mathcal{H}}$ for which the time evolution is described by a unitary time-evolution is said to be **complete**.

Remark 5.7.2. In this way, a self-adjoint Hamiltonian gives rise to a unitary time-evolution by Theorem 5.3.3. If the Hamiltonian is not self-adjoint, it may have infinitely many self-adjoint extensions. If it has a unique self-adjoint extension, then for convenience we will also say that the quantum system described by it is complete.

From the calculations above, it follows that the quantum Kepler problem is complete for dimensions $d \geq 4$. In one, two and three dimensions there are infinitely many choices. Our expectation that the lower the dimension, the more there is to choose, turns out to be true.

In the physics literature, the hydrogen atom in three dimensions is often solved in the way given in [12, 21]. Nothing is mentioned about the self-adjoint extension that is chosen. However, implicitly an extension is chosen by the method of solution. Indeed, they assume that the wave functions can be smoothly extended to the origin, so in fact the initial domain that is chosen for the Hamiltonian is $C_0(\mathbb{R}^3)$ rather that $C_0(\mathbb{R}^3 \setminus \{0\})$. We have

$$\begin{aligned} \|V\psi\|^2 &= \int_{\mathbb{R}^3} \frac{|\psi(x)|^2}{|x|^2} dx \\ &= \int_0^{2\pi} \int_0^{\pi} \int_0^{\infty} |\tilde{\psi}(r,\theta,\phi)|^2 dr \sin\theta d\theta d\phi \\ &< \infty, \end{aligned} \tag{5.8}$$

which justifies the extension of the domain. By the Kato-Rellich theorem [9, Theorem 6.1.8], the operator $(\hat{H}, C_0(\mathbb{R}^3))$ is essentially self-adjoint. This choice corresponds to the Dirichlet boundary conditions, and hence to $\lambda = 0$.

Remark 5.7.3. This method of extending the operator to the smooth functions on the whole $\mathbb{R}^d$ only works for $d \geq 3$. However, for $d \geq 4$, we already proved the stronger result that $\hat{H}$ is essentially self-adjoint on $C_0^\infty(\mathbb{R}^d \setminus \{0\})$.

In the next chapter, we will discuss the quantum analogue of Moser's treatment and come back to the question of choosing self-adjoint extension. In particular, we will address the question which explicit extension is chosen in the Fock approach.

Chapter 6

Quantum Kepler problem

In this chapter, solving the quantum Kepler problem refers to any way to obtain the spectrum of the Hamiltonian of the hydrogen atom together with the corresponding electron distributions. The most important aim of this chapter is to discuss Fock's treatment of the hydrogen atom. Although this was done thirty-four years earlier, it can be considered as the quantum analogue of Moser's work. In this case, we look at what we call the Schrödinger quantization of the Kepler problem, as described in Chapter 5, and we will apply our general method of interchanging the position and momentum coordinates and then apply a stereographic projection. However, we start with Pauli's abstract method to obtain the spectrum of the hydrogen atom, because it was the first theoretical derivation of the spectrum, without calculating the corresponding electron wave functions. We will also explain the relations to the rest of the chapter later. The quantization procedure here is often called canonical quantization.

6.1 Spectrum obtained by Lie algebra representations

In 1926, Pauli gave the first quantum mechanical treatment of the hydrogen atom [29]. He derived its negative energy spectrum by means of calculations with operators and commutators. Later, his method was understood in terms of Lie algebras, as described by Bander and Itzykson [3]. They also described the method for positive energies in [4]. We treat this method here in terms of Lie algebra theory, but we leave out most of the proofs and calculations leading to the technical results.

Pauli's article treats the three-dimensional Kepler problem. We think that the method can be generalized to d dimensions in a straightforward way, but the representation theory will be more difficult in other cases, so we only decribe the three-dimensional case here.

Suppose that the position operator q and the momentum operator p are self-adjoint operators[1] on some Hilbert space $\mathcal{H}$ representing the three-dimensional space, corres-

[1]The classical counterparts of these operators in three dimensions are denoted in boldface.

ponding to the physical situation of a particle of mass 1 in a Kepler potential. They are subjected to the following (Heisenberg) commutation relations:

$$\begin{aligned} [q_i, q_j] &= [p_i, p_j] = 0, \\ [q_i, p_j] &= i\hbar\delta_{ij}. \end{aligned} \tag{6.1}$$

Remark 6.1.1. We treat these observables as mere algebraic objects and apply (Lie) algebraic methods to them. We do not refer to the explicit Hilbert space, on which these operators are initially unbounded, closable and densely defined, and where functional analytic comments are needed.

According to the recipe of canonical quantization we quantize the Hamiltonian H and the angular momentum vector $\mathbf{L}$ by just replacing the position and momentum vectors occurring in their expression by the corresponding operators. For the Hamiltonian we obtain:

$$\hat{H} = \frac{p^2}{2} - \frac{k}{\|q\|},$$

where $p^2 = \sum_{i=1}^{3} p_i^2$. These expressions are algebraically well-defined. The other important quantity needed for the description of the hydrogen atom is the quantization of the Runge-Lenz vector, classically given by $\mathbf{K} = \mathbf{p} \times \mathbf{L} - \frac{k\mathbf{q}}{\|q\|}$. This expression, however, cannot be quantized just by replacing classical position and momentum by their quantum analogues, since there would be an ambiguity in the cross product. Indeed, should we take $p_2L_3 - p_3L_2$ or $L_3p_2 - L_2p_3$ for the first component of $\mathbf{p} \times \mathbf{L}$? These operators are not the same, which follows from the commutation relations of p and L.

Pauli solved this by quantizing the expression:

$$\mathbf{K} = \frac{1}{2}(\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}) - \frac{k\mathbf{q}}{\|q\|}.$$

Classically, this expression is the same as the original definition, but the ambiguity in quantum mechanics now vanishes.[2]

It turns out to be useful to use the Levi-civita symbol in the description of a cross product. The Levi-Civita symbol ε_{ijk} is the totally anti-symmetric tensor. If $\mathbf{a} = \mathbf{b} \times \mathbf{c}$, we write:

$$a_i = \sum_{j,k} \varepsilon_{ijk} b_j c_k.$$

Remark 6.1.2. This is a convention rather than merely an agreement on notation, since we also decide in which order the cross product should be taken. In this definition of the cross product, there is no ambiguity.

[2]The ambiguity can also be removed by writing $\mathbf{p} \times \mathbf{L} = \mathbf{p} \times (\mathbf{q} \times \mathbf{p}) = \|\mathbf{p}\|^2\mathbf{q} - \langle \mathbf{p}, \mathbf{q} \rangle \mathbf{p}$ in the classical case and quantizing this expression, which yields an unambiguous quantization.

Proposition 6.1.3. Next to the Heisenberg commutation relations given in equation (6.1), the angular momentum and the Runge-Lenz vector are conserved, i.e.

$$[\hat{H}, L_i] = 0, \qquad [\hat{H}, K_i] = 0,$$

and the following commutation relations hold:

$$\begin{aligned}
[q_i, L_j] &= i\hbar \sum_k \varepsilon_{ijk} q_k, \qquad [p_i, L_j] = i\hbar \sum_k \varepsilon_{ijk} p_k, \\
[L_i, L_j] &= i\hbar \sum_k \varepsilon_{ijk} L_k, \qquad [L_i, K_j] = i\hbar \sum_k \varepsilon_{ijk} K_k, \\
[K_i, K_j] &= i\hbar \sum_k \varepsilon_{ijk} (-2\hat{H}) L_k,
\end{aligned}$$

for all $i, j \in \{1, 2, 3\}$.

Proof. The first two relations follow from the conservation of $\mathbf{L}$ and $\mathbf{K}$ in the classical case. The other relations are the result of explicit calculations. We use the fact that $\frac{1}{\|q\|}$ is rotationally invariant and hence commutes with the angular momentum operator. □

Proposition 6.1.4.

$$\sum_{i=1}^{3} L_i K_i = \sum_{i=1}^{3} K_i L_i = 0.$$

A proof is obtained by calculation. These relations also hold in the classical case. However, note that in the quantum case, we need to check both relations, whereas in the classical case checking one of them suffices because of the commutativity of the scalar product. In the quantum case, the expression given above does not define an inner product.

In the case of the length of the Runge-Lenz vector we have a "quantum correction" in the following way, as follows from explicit calculation.

Proposition 6.1.5.

$$\|K\|^2 = 2\hat{H}(\|L\|^2 + \hbar^2) + k^2. \tag{6.2}$$

In what follows, we will determine the energy spectrum of the hydrogen atoms by identifying the eigenspaces with Lie algebra representations using the relations derived above. To this end, we distinguish the different signs of E, leaving out the case $E = 0$. First, however, we need to discuss the concept of natural degeneracy, because this gives a correct interpretation of the spectrum and its degeneracy in terms of unitary irreducible representations of the Lie algebra corresponding to the infinitesimal symmetries of the system.

6.1.1 Natural degeneracy

It turns out that the spectrum of many Hamiltonian operators can be determined and examined by means of Lie algebra theory. The eigenspaces corresponding to elements of the spectrum, both in the discrete and in the continuous one, can be identified with unitary irreducible representations. This method also contains some aspects of the problem of degeneracy, since the multiplicity of the representation equals the spectral degeneracy in the case of a discrete spectrum. It is well-known that this is more subtle for the continuous spectrum, but the method still accounts for the elements of the spectrum.

If a degeneracy comes up "coincidentally", i.e. without any obvious reason, it is often referred to as **accidental degeneracy**. This notion is not very well defined.

In many cases, there is reason to believe that degeneracy is not accidental, but due to a certain hidden symmetry of the system. Thus, the system is **naturally degenerate**. To this end, the higher-dimensional eigenspaces corresponding to some element of the discrete spectrum are identified with the unitary irreducible representations of some infinitesimal symmetry group of the system. More about this is written in [23]. We apply this idea to the hidden symmetries of the Kepler problem. We determine the dimension of $\mathcal{H}_E$ for any nonzero value of E. Indeed, the well-known results will follow.

6.1.2 Negative Energies

Let $E < 0$. The operators L and K together with their commutation relations can be identified with a Lie algebra in the following way.

Proposition 6.1.6. The operators L and K span a six-dimensional Lie algebra isomorphic to $i\mathfrak{su}(2) \oplus i\mathfrak{su}(2)$.

Proof. Define the following operators:

$$I := \frac{1}{2}(L + (-2E)^{-\frac{1}{2}}K),$$
$$J := \frac{1}{2}(L - (-2E)^{-\frac{1}{2}}K).$$

For I and J, the following commutation relations hold:

$$[I_i, I_j] = i\hbar \sum_k \varepsilon_{ijk} I_k,$$
$$[J_i, J_j] = i\hbar \sum_k \varepsilon_{ijk} J_k,$$
$$[I_i, J_j] = 0,$$

for all $i, j \in \{1, 2, 3\}$. This is checked by writing out the commutation relations. Using the obervations $I^* = I$ and $J^* = J$, we conclude that I and J span a Lie algebra isomorphic to $i\mathfrak{su}(2) \oplus i\mathfrak{su}(2)$. Note that the scalar multiplication of both summands with i is because of the self-adjointness of I and J. □

Following to the idea of natural degeneration, we assume that $\mathcal{H}_E$ is isomorphic to a unitary irreducible representation of $i\mathfrak{su}(2) \oplus i\mathfrak{su}(2)$.

The unitary irreducible representations of $i\mathfrak{su}(2) \oplus i\mathfrak{su}(2)$ are given by the tensor products $L(m) \otimes L(n)$ for some natural numbers m, n [17]. Here, $L(n)$ denotes the irreducible representation of $\mathfrak{sl}(2)$ of highest weight n. We conclude that

$$\{\psi \in \mathcal{H} | \hat{H}\psi = E\psi\} \cong L(m) \otimes L(n)$$

for some $m, n \in \mathbb{N}_0$. The first factor corresponds to the Lie algebra spanned by the I_i's and the second to the Lie algebra spanned by the J_i's.

The elements I^2 and J^2 are the Casimir operators of their corresponding summands of $i\mathfrak{su}(2) \oplus i\mathfrak{su}(2)$. Hence, the following holds:

$$I^2|_{L(m)\otimes L(n)} = m(m+2)\frac{\hbar^2}{4},$$
$$J^2|_{L(m)\otimes L(n)} = n(n+2)\frac{\hbar^2}{4},$$

There is also a relation between the two Casimir operators, as follows from the following calculations:

$$\begin{aligned} I^2 - J^2 &= \frac{1}{2}(\langle I+J, I-J\rangle + \langle I-J, I+J\rangle \\ &= \frac{1}{2}(-2mE)^{-\frac{1}{2}}(\langle K, L\rangle + \langle L, K\rangle) = 0. \end{aligned}$$

We conclude that $m = n$. Hence

$$\{\psi \in \mathcal{H} | \hat{H}\psi = E\psi\} = L(n) \otimes L(n)$$

for some $n \in \mathbb{N}_0$.

Note that on $L(n) \otimes L(n)$ we have $L^2 + (-2E)^{-\frac{1}{2}}K^2 + \hbar^2 = 2(I^2 + J^2) = n(n+2)\hbar^2 + \hbar^2 = (n+1)^2\hbar^2$. Luckily, we can rewrite equation (6.2) as

$$L^2 + (-2E)^{-\frac{1}{2}}K^2 + \hbar^2 = -\frac{k^2}{2E},$$

from which we obtain the possible energy levels:

$$E_n = -\frac{k^2}{2(n+1)^2\hbar^2}.$$

Since the dimension of $L(n)$ is $n+1$, it follows that $\dim \mathcal{H}_{E_n} = (n+1)^2$, so the energy levels are degenerate with multiplicity $(n+1)^2$.

6.1.3 Positive Energies

Let $E > 0$. The operators L and K together with their commutation relations can be identified with a Lie algebra in the following way.

Proposition 6.1.7. The operators L and $\tilde{K} = (\frac{\mu}{2E})^{\frac{1}{2}}K$ span a six-dimensional Lie algebra isomorphic to $i\mathfrak{o}(3,1)$.

Proof. The commutation relations of L and $\tilde{K}$ show that these operators generate the Lorentz algebra $i\mathfrak{o}(3,1)$ [4, 26]. □

According to the idea of natural degeneration, we assume that $\mathcal{H}_E$ can be identified with a unitary irreducible representation of $i\mathfrak{o}(3,1)$.

The unitary irreducible representations of $i\mathfrak{so}(3,1)$ are given by the spherical representations S_s, labelled by a complex number s, as described in Section 3.6. So we have

$$\{\psi \in \mathcal{H} \mid \hat{H}\psi = E\psi\} = S_s$$

for some $s \in \mathbb{C}$ such that either $\Re(s) = \frac{d-1}{2}$ or $0 < s < d-1 = 2$.

Using the fact that $\tilde{K}^2 - L^2$ acts as a Casimir operator corresponding to the scalar $-\hbar^2 s(s-2)$ for the representation labelled by s, it follows from equation (6.2) that

$$H = \frac{k^2}{2(\tilde{K}^2 - L^2 - \hbar^2)} = -\frac{k^2}{2\hbar^2(s-1)^2}.$$

From this, it follows that we are in the case $0 < s < 2$, since the Hamiltonian is an observable.

Remark 6.1.8. The degeneration is according to the representation theory of the Lorentz algebra. However, in the positive case we cannot say anything about the "multicplicity" of a representation, since the positive spectrum is continuous. However, notice that two s-values, namely an arbitrary s-value and its mirror image in 1, yield a representation with the same energy.

Remark 6.1.9. The reason that the derivation of the spectrum for positive energies seems shorter than the one for negative energies is that we do not need to introduce new operators that come up as the actual generators of the Lie algebra for positive energies. However, we did not perform the calculations to check if L and K really generate the Lorentz algebra, but we want to make the idea of the method clear rather than its technical details.

6.2 Spaces of constant curvature

In this section, we describe the method by Fock [11] to solve the quantum Kepler problem. It can be considered the quantum analogue of Moser's method, which we described in Section 4.3. It is remarkable that the article by Fock was published thirty-five years earlier than its classical analogue. In this section, we describe its general idea in d dimensions. After this section, we also give Bargmann's comments on the relation between this method and the method by Pauli, of which we gave a modern descrption in Section 6.1. Fock only considered the negative energy case in detail and mentions

very little about postitive energies. Bander and Itzykson gave a modern treatment of Fock's work in 1966 [3] and also accounted for positive energies [4]. We also describe this.

We consider the d-dimensional quantum Kepler problem, which is given by the (time-independent) Schrödinger equation $\hat{H}\psi = E\psi$, where $\hat{H}$ denotes the Hamilton operator of the Kepler problem, which is some self-adjoint extension of $\hat{H} = -\frac{\hbar^2}{2\mu}\Delta_{\mathbb{R}^d} - \frac{k}{\|q\|}$, which is initially defined on $C_0(\mathbb{R}^d \setminus \{0\})$. For now, we do not need to specify this extension. The Schrödinger equation is given by:

$$(-\frac{\hbar^2}{2\mu}\Delta_{\mathbb{R}^d} - \frac{k}{\|q\|})\psi(q) = E\psi(q). \tag{6.3}$$

Fock solves this equation by transforming it to momentum space (by a Fourier transform), and then applying a stereographic projection to the sphere for $E < 0$. Bander and Itzykson showed that for $E > 0$ it is possible to do the same by performing a stereographic mapping to the hyperboloid. We will point out that the problem is solved by spherical functions. The method fits in the general idea of interchanging the position and momentum coordinates, which is in the quantum case done by a Fourier transform, and then apply a stereographic projection, just as we did in the Moser case.

Definition 6.2.1. The Fourier transform from position space to momentum space in quantum mechanics is given by:

$$\hat{\psi}(p) = A_d \int_{\mathbb{R}^d} \psi(q) \exp(-\frac{ip \cdot q}{\hbar}) dq. \tag{6.4}$$

Remark 6.2.2. Here A_d is a normalisation constant, which does not bother us, because we transform both sides of an equation, so that these constants cancel. We choose to not specify it, because there are different conventions for it.

To calculate the Fourier transform[3] of equation (6.3), we recall that the Laplacian with respect to q of a function corresponds to multiplication with $\|p\|^2$ and that the Fourier transform of $\frac{1}{\|q\|}$ is given by $2^{d-1}\pi^{\frac{d-1}{2}}\Gamma(\frac{d-1}{2})\|p\|^{-(d-1)}$. Using the formula $\mathcal{F}(fg) = \frac{1}{(2\pi)^d}\mathcal{F}(f) * \mathcal{F}(g)$ with respect to $\frac{k}{\|q\|}\psi(q)$, we obtain the following result.

Proposition 6.2.3. The Kepler Schrödinger equation in momentum space is given by

$$\frac{1}{2}(\|p\|^2 - 2\mu E)\hat{\psi}(p) = C_d \int_{\mathbb{R}^d} \frac{\hat{\psi}(p')}{\|p - p'\|^{d-1}} d^d p', \tag{6.5}$$

where $C_d = \frac{\mu k \Gamma(\frac{d-1}{2})}{2\pi^{\frac{d+1}{2}}\hbar}$.

Remark 6.2.4. We will look for L^2 solutions $\hat{\psi}$ of this Fourier transformed Schrödinger equation. From these, by applying the inverse Fourier transform, we recover the wave functions as function of q.

[3]Note that it is not yet necessary to distinguish between $E < 0$ and $E > 0$.

Definition 6.2.5. We define the m^{th} **Sobolev space** $W^m(\mathbb{R}^d)$ to be the space of functions $f \in L^2(\mathbb{R}^d)$ such that the function $p \mapsto (ip)^n(\mathcal{F}f)(p) \in L^2(\mathbb{R}^d) \forall n \in \{1, \ldots, m\}$, i.e.

$$W^m(\mathbb{R}^d) := \{f \in L^2(\mathbb{R}^d) \,|\, p \mapsto (ip)^n(\mathcal{F}f)(p) \in L^2(\mathbb{R}^d) \forall n \in \{1, \ldots, m\}\}. \tag{6.6}$$

Remark 6.2.6. This definition generalizes to the concept of differentiation on $\mathbb{R}^d$, since the Fourier transform intertwines differentiation and multiplication by the independent variable. There are more general definitions of Sobolev spaces. E.g., one does not need to restrict to $\mathbb{R}^d$ and it turns out to be possible and useful to define non-integer Sobolev spaces.

The following result relates the previous chapter on self-adjoint extensions of the quantum Kepler Hamiltonian to the quantization presented in this section. Indeed, if we look for solutions of the Schrödinger equation, we need a self-adjoint Hamiltonian in order to have a complete theory. In the text by Fock, this choice is not explicitly made. However, it is made implicitly, as follows from the next theorem. We use the fact that the quantum Fourier transform is a unitary transformation from the L^2 functions of q to the L^2 functions of p.

Theorem 6.2.7. The self-adjoint extension of the Hamiltonian automatically chosen in the generalized Fock method is

- the unique one for $d \geq 4$;
- the unique one for initial domain $C_0^\infty(\mathbb{R}^3)$.

Proof. For $d = 4$, the claim is obvious. For $d = 3$, we know that the inverse Fourier transformed wave functions are L^2. Therefore, in particular all functions of $C_0^\infty(\mathbb{R}^3)$ are in the domain of the self-adjoint extension. For every domain of the symmetric Schrödinger equation that contains these functions, the named self-adjoint extension is the unique one. □

Remark 6.2.8. From this we conclude that indeed the generalized Fock method describes the same physics as the usual way of solving the hydrogen Schrödinger equation. The steps in the next sections, which give an explicit way of finding the solutions of the Fourier transformed Schrödinger equations are analytically harmless.

Remark 6.2.9. The one-dimensional case is not included in the generalized Fock method. There are still choices to be made in the two-dimensional case. We did not manage to obtain an explicit result about the latter case. In particular, the three-dimensional choice is interesting physically. The choice made also corresponds to the usual choice in which the wave functions are continuously extended, which was described in the previous chapter.

We will now distinguish between both energy signs and apply a stereographic projection.

6.2.1 Negative Energies

Suppose $E < 0$. We search for the negative spectrum and the corresponding eigenvalues of the Schrödinger equation (6.5). We map the equation to an equation on S^d. We follow both [3] and [7], but use the notation of the latter, since this is more elegant.

Proposition 6.2.10. Let $p_0 = \sqrt{-2\mu E}$ and set $p_j = p_0 x_j$ for $j = 1, \dots, d$. We embed the space $\mathbb{R}^d$ with coordinates x_j into $\mathbb{R}^{d+1}$ with coordinates X_j by a stereographic projection of the sphere, i.e.

$$X_j = \frac{2x_j}{\|x\|^2 + 1},$$
$$X_{d+1} = \frac{\|x\|^2 - 1}{\|x\|^2 + 1},$$

for $j = 1, \dots, d$. Then, setting $\Psi(X) = \frac{1}{\sqrt{p_0}} \left(\frac{\|p\|^2 + p_0^2}{2p_0} \right)^{\frac{d+1}{2}} \hat{\psi}(p)$, equation (6.5) is equivalent to the following integral equation:

$$C_d \int_{S^d} \frac{\Psi(X')}{\|X - X'\|^{d-1}} d\Omega'_d = p_0 \Psi(X). \tag{6.7}$$

A proof is obtained by straightforward, but tedious calculations, as is performed in [7]. Note that from the stereographic projection, the explicit form of the volume form follows, which is needed for the calculation. We may interpret this integral equation as an eigenvalue equation with spectral parameter $p_0 > 0$ instead of $E < 0$.

Proposition 6.2.11. The group $\mathrm{O}(d+1)$ is a symmetry group of the quantum Kepler problem.

Proof. If $A \in \mathrm{O}(d+1)$, then we see that if $\Psi(X)$ satisfies equation , then also $\Psi(OX)$ satisfies this equation, since the domain of integration, $\frac{1}{\|X - X'\|^{d-1}}$ and $d\Omega'_d$ are invariant under O. □

Remark 6.2.12. This result is really important. Inherent to the quantization method and the implicit choice of the self-adjoint extension, the problem is regularized in some sense. Therefore, in the quantum case, the global symmetry is obtained automatically. In the classical case, we needed to explicitly regularize the problem before we were able to determine the richer global symmetry.

In the case of the negative spectrum, which is discrete, we can use the virial theorem [9, Theorem 6.2.8] to conclude the following.

Lemma 6.2.13 (Virial theorem)**.** The expectation values $\langle E \rangle$ and $\langle T \rangle$ of the energy E and the kinetic energy T in the case of negative energy are related according to:

$$\langle E \rangle = -\langle T \rangle.$$

Remark 6.2.14. The Virial theorem is true for Hamiltonians with some special properties. It must be relatively bounded with respect to the Laplacian. We cannot use this result for the continuous spectrum.

Proposition 6.2.15. The map given by $\hat{\psi}(p) \mapsto \Psi(X)$ corresponding to some fixed E preserves scalar products.

Proof. If we invoke the Virial theorem of quantum mechanics, stated as Lemma 6.2.13, we conclude that:

$$E \int_{\mathbb{R}^d} \|\hat{\psi}(p)\|^2 d^d p = -\int_{\mathbb{R}^d} \frac{p^2}{2\mu} \|\hat{\psi}(p)\|^2 d^d p.$$

We use this to obtain:

$$\begin{aligned}\int_{S^d} \|\Psi(X)\|^2 d\Omega_d &= \int_{\mathbb{R}^d} \frac{\|p\|^2 + p_0^2}{2p_0^2} \|\hat{\psi}(p)\|^2 d^d p \\ &= \int_{\mathbb{R}^d} \frac{-2\mu E}{2(-2\mu E)} \|\hat{\psi}(p)\|^2 d^d p + \frac{1}{2} \int_{\mathbb{R}^d} \|\hat{\psi}(p)\|^2 d^d p \\ &= \int_{\mathbb{R}^d} \|\hat{\psi}(p)\|^2 d^d p.\end{aligned}$$

So the map $\hat{\psi}(p) \mapsto \Psi(X)$ is a linear isometry, which proves the claim. □

Corollary 6.2.16. The map $\hat{\psi}(p)$ composed with the quantum Fourier transform with A_n (cf. equation (6.4)) chosen such that the Fourier transform is an isometry, extends to a unitary map $\mathcal{T} : \mathcal{H} \to L^2(S^d)$, where $\mathcal{H}$ denotes the completion of the pre-Hilbert space of (infinite) linear combinations of eigenfunctions corresponding to negative eigenvalues of the Kepler Hamiltonian to $L^2(S^d)$.

Remark 6.2.17. It is well-known [21] that the eigenfunctions corresponding to different eigenvalues of the Kepler Hamiltonian are orthogonal. The same holds for solutions of equation (6.2.1).

In what follows, we refer to [3, 7] for the details. It is known that equation (6.2.1) is solved by spherical harmonics, since:

$$\frac{\Gamma(\frac{d-1}{2})}{2\pi^{\frac{d+1}{2}}} \int_{S^d} \frac{Y_l(X')}{\|X - X'\|^{d-1}} d\Omega'_d = \frac{2}{d-1+2l} Y_l(X).$$

Because the set of spherical harmonics is complete, we have also found all eigenvalues of the Kepler Hamiltonian because of the one-to-one unitary correspondence $\mathcal{T}$. We can calculate the energy spectrum by comparing equations (6.3) and (6.2.1):

$$\frac{\hbar}{\mu k} \sqrt{-2\mu E} = \frac{2}{d-1+2l},$$

from which it follows that:

$$E_l = -\frac{2\mu k^2}{\hbar^2 (d-1+2l)^2},$$

with $l = 0, 1, 2, \ldots$. Note that the energy levels also depend on the dimension d. Each eigenvalue has multiplicity $\frac{(d+2l-1)(d+l-2)!}{(d-1)!l!}$. In three dimensions, this corresponds to the well-known formula:

$$E_l = -\frac{\mu k^2}{\hbar^2 (l+1)^2}.$$

Remark 6.2.18. We have proved that the set of solutions of the d-dimensional Kepler Schrödinger equation is unitary equivalent to the set of $d+1$-dimensional spherical harmonics. The latter must not be confused with the spherical harmonics one obtains by solving the Kepler Schrödinger equation by separation of variables. They arise in a totally different way.

6.2.2 Positive Energies

Suppose $E > 0$. We search for positive elements of the spectrum.

Remark 6.2.19. We cannot do this in exactly the same way as for the negative energies, because the positive spectrum is continuous, and hence technically more difficult. E.g., it is not possible to look for eigenvalues in the same way as for a discrete part of the spectrum. We follow [4].

In the positive spectrum case, the map to the hyperboloid integral equation is done in a similar way as in the negative one, but we divide it in two steps.

Proposition 6.2.20. Let $p_0 = \sqrt{2\mu E}$ and set $p_j = p_0 x_j$ for $j = 1, \ldots, d$. Define $\phi(x) = \hat{\psi}\psi(p)$. Then equation (6.5) is equivalent to:

$$\frac{1}{2}(\|x\|^2 - 1) = \frac{C_d}{(2\mu E)^{-\frac{1}{2}}} \int \frac{\phi(x')}{\|x - x'\|^2} d^d x'$$

This result can be verified in a straightforward way.

Proposition 6.2.21. Let us embed the space $\mathbb{R}^d$ with coordinates x_j into $\mathbb{R}^{d,1}$ with coordinates X_j by a stereographic projection of the two-sheeted hyperboloid, i.e.

$$X_j = \frac{2x_j}{1 - \|x\|^2},$$
$$X_{d+1} = \frac{1 + \|x\|^2}{1 - \|x\|^2},$$

for $j = 1, \ldots, d$. Then, setting $\Psi(X) = \|1 - X_{n+1}\|^{-\frac{d+1}{2}} \phi(x)$, equation (6.5) is equivalent to:

$$\Psi(X) = -\frac{C_d \varepsilon(X_{n+1})}{(2\mu E)^{-\frac{1}{2}}} \int_{F^n} \frac{\Psi(X')}{\|(\|X - X'\|_L^2)\|^{\frac{d-1}{2}}} d\Omega'_d,$$

where $\varepsilon(X_{n+1})$ denotes the function that is equals 1 for $X_{n+1} \geq 1$ and -1 for $X_{n+1} < 1$. This function assigns a sign to every sheet of the hyperboloid.

The proof consists of straightforward, but tedious calculations.

Proposition 6.2.22. The group $O(d,1)$ is a symmetry group of the quantum Kepler problem for positive energies.

The proof is analogous to the proof of Proposition 6.2.11.

Remark 6.2.23. The equation we turned the problem into is of the same type as for negative energies. However, we cannot proceed in the same way now. E.g., the Virial Theorem does not hold for the continuous spectrum. The problem can analytically be solved by a lot of calculations. Cf. [4] for the details. They indeed find the well-known positive spectrum in the three-dimensional case.

6.3 From Pauli to Fock

The approaches of Pauli and Fock both calculate the spectrum. Fock's approach yields more results. Indeed, the wave functions are also calculated and he accounts for the global symmetry of the quantum Kepler problem, where Pauli only accounts for infinitesimal symmetries of the system. Bargmann showed that both treatments are closely related to each other by explaining how Pauli's method fits into Fock's one [5]. We will briefly describe this. To this end, we restrict ourselves to the three-dimensional case of Fock's treatment, since we treated only the three-dimensional case of the Pauli method because of its simplicity. We also only treated the negative energy case. We think, however, that a generalization of Pauli's method, as well as of Bargmann's comments, can be obtained in a straighforward way, but it would need some calculations.

Recall that an infinitesimal rotation acting on a function f is a linear combination of terms of the form

$$D_{ij}f = y_i\frac{\partial f}{\partial y_j} - y_j\frac{\partial f}{\partial y_i}.$$

In particular, Pauli's angular momentum operators L_i are of this form, since $p_i = -i\hbar\frac{\partial}{\partial q_i}$. He shows that these operators, and the Runge-Lenz vector operators K_i, commute with the Hamiltonian, and can hence be considered as quantum integrals of motion. We treated this too, and we also gave the other commutation relations in Section 6.1. We now come to the idea of Bargmann. To this end, we change notation from the usual L_i's to

$$L_{ij} = q_ip_j - q_jp_i.$$

Definition 6.3.1. Define anti-symmetric U_{ij} and V_{ij} with $1 \leq i,j \leq 3$ operators by:

$$U_{ij}f = V_{ij}f = -i\hbar L_{ij} = p_i\frac{\partial f}{\partial p_j} - p_j\frac{\partial f}{\partial p_i},$$

$$V_{4i}f = U_{4i}f + 2\frac{p_i}{p_0}f = -\frac{ik\mu}{\hbar}K_if$$

U_{ij} and V_{ij} satisfy the commutation relations of infinitesimal rotations. If $V_{ij}g = 0$ for some test function g, then

$$V_{ij}\psi = gU_{ij}(\frac{\psi}{g}),$$

where we use the relation $V_{ij}(fg) = g(U_{ij}f) + f(V_{ij}g)$, which is verified by calculation. From this it follows that $g \propto (p_0^2 + p^2)^{-2}$. Define $\Phi = C(p_0^2 + p^2)^2\psi$. Then

$$V_{ij}\psi = C^{-1}(p_0^2 + p^2)^{-2}U_{ij}\Phi,$$

which has the form of an infinitesimal transformation. The idea is to look for functions $\xi_1, \ldots, \xi_4$ as functions of $p_1, \ldots, p_3$ which perform an infinitesimal rotation if U_{ij} acts on them. Bargmann observed that these functions are given by

$$\xi_i = \frac{2p_0p_i}{p_0^2 + p^2},$$
$$\xi_4 = \frac{p_0^2 - p^2}{p_0^2 + p^2},$$

which are exactly the coordinates of the stereographic projection. This means that the infinitesimal rotations of the three-dimensional sphere obtained by the stereographic projection are given by the integrals of motion obtained in Pauli's treatment. This exhibits a close relation between the two approaches.

Remark 6.3.2. Bargmann also remarks that the positive energy case can be considered in an analogous way.

Chapter 7

Outlook

As said earlier, much work has been done on the Kepler problem. A small part of it, namely the results that have to do with the Moser and Fock treatments of regularization and quantization, is described in this text, and we hope to have explained some new connections and relations as well as some analogues between the classical and the quantum case.

One question is how the relation between Moser and Ligon-Schaaf is described in quantum theory. In particular, what the time-relation between arclength s and real time t translates to in the quantum case.

Another problem is to understand the regularization and quantization in terms of the Plancherel Theorem. This was the author's original thesis project, but eventually this project went in another direction.[1] The original idea was to relate the spectral problem corresponding to the Kepler problem, i.e. the Schrödinger equation, to a spectral problem on the sphere and the hyperboloid and relate and explain their similarities. This is still an open question.

[1] In particular the work concerning the self-adjoint extensions of the quantum Kepler Hamiltonian and their relations to Fock's method were not planned at the start.

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