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Hidden Symmetries of the Kepler Problem in n Dimensions

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Abstract

This thesis focuses on the Kepler problem describing the motion of a particle under the influence of a central force according to an inverse-square law. A short review of the problem – as treated in standard (quantum) mechanics courses – is followed by an analysis of the underlying hidden symmetries. The main aim of this text is to study the n-dimensional generalisation of the Kepler problem, its solutions as well as the corresponding symmetry groups. This is realised by following to the ideas of Vladimir Fock where a Fourier transform on the Schrödinger equation associated to the quantum Kepler problem is considered, to then apply a stereographic projection. In this text an emphasis is put on the role quantum mechanical operators play in symmetry as a fundamental underpinning. In doing so, the framework of Lie groups and Lie algebras is introduced and employed.

Acknowledgements

First and foremost, I would like to express my gratitude to dr. T.F. Görbe for his invaluable e□ort in guiding and encouraging me throughout the project. I truly admire his enormous enthusiasm and expertise. Our weekly meetings and the extensive feedback provided on many of my drafts have been extremely helpful to me. Moreover, I would like to thank prof.dr. R.I. van der Veen on agreeing to be my second assessor.

Contents

Introduction

Throughout history, there has always been a fascination about celestial bodies in our solar system. In particular, the study of planets goes back at least to ancient Greek astronomy. Forging ahead to the 16^{th} and 17^{th} century, there was made substantial, even revolutionary, progress in the field of astronomy due to the work of Johannes Kepler and Isaac Newton. They contributed by providing empirical laws about planets and its theoretical underpinnings, respectively. One was now able to accurately describe the motion of bodies in the solar system, an enormous achievement. Most importantly, it came to light that, when considering two bodies, the first body exerts a gravitational force on the other body and vice versa. Newton described this force in mathematical terms, which turned out to be proportional to the inverse square of the distance between two bodies. That is, the respective motion follows an inverse-square law. Going beyond the scope of celestial bodies, there are other systems where the motion is subject to an inverse-square law. The modelling of motion of such systems is referred to as the Kepler problem.

In this thesis, we consider the Kepler problem with both a classical mechanical approach, as well as a quantum mechanical one. We describe the symmetries in both frameworks with an emphasis on the latter. First of all, in classical mechanics we shall look at various conserved quantities. Well-known are the conservation of energy and angular momentum. But it turns out there is another conserved quantity one can find, the Laplace-Runge-Lenz vector. These conserved quantities are a result of symmetries, which are hence arguably more fundamental. One speaks of symmetry within a system if the dynamics of that system are found to be invariant under a transformation, or a class thereof. An example of a symmetry a system can possess is rotational symmetry, where the system does not behave any different, in the dynamical sense, after rotation. We elaborate in this thesis on the various symmetries observed in the classical Kepler problem, where we in particular describe an unexpected one, which we shall refer to as hidden symmetry.

The main focus of this text is, however, not on classical mechanics. Instead, after reviewing symmetries in that setting, we shift to the quantum mechanical framework with the aim of ultimately elucidating on the symmetries of the quantum Kepler problem in an arbitrary dimension. Because it is instructive to initially inspect what key elements are at play in three dimensions, we do treat this case extensively. The quantum Kepler problem for three dimensions is best modelled by the hydrogen atom, where the proton and electron are subject to Coulomb's force which, indeed, follows an inverse-square law. We note that quantum mechanically, motion is described by the wave function which is in turn governed by Schrödinger's equation. Of main importance at this level are

the commutation relations of operators. They allow us to pave a road in drawing the analogue of conserved quantities established in classical mechanics. This, in turn, allows us to arrive at symmetries of the hydrogen atom by viewing these commutation relations in the context of Lie algebras.

The argument involved in generalising the Kepler problem to an arbitrary dimension comes packed with notions of Fourier transforms and stereographic projections, devoting our treatment to the reasoning of Vladimir Fock and the generalisation thereof in an article by Bander and Itzykson. The goal is look at whether the hidden symmetry survives the generalisation process of going to an arbitrarily picked dimension.

It is important to remark on what this thesis is *not*. This thesis is not written with the intention of showing new results. We instead review existent literature. The Kepler problem in itself is quite well-studied, however, the generalisation to any dimension remains a far lesser known area.

We believe that readers of this text with a mathematical background will appreciate the fundamental role mathematics plays in the of the quantum Kepler problem generalised with regard to its dimension. On the other hand, those with a background in physics might find it enjoyable to see concepts they know by heart at a rather foundational level.

Chapter 1

The Classical Kepler Problem

The classical Kepler problem is regarded as one of the most fundamental problems in the realm of classical mechanics. It is named after the German mathematician and astronomer Johannes Kepler (1571–1630), who lived in Graz, Austria, from which he and his family would get ultimately banished. Kepler made revealing and influential contributions in the field of astronomy, making him a key contributor in the scientific revolution of the 16^{th} and 17^{th} centuries.

His scientific career experienced quite a surge in the year 1600 when the Danish astronomer Tycho Brahe (1546–1601) invited Kepler to his newly constructed observatory near Prague. Whereas most astronomers in that era where trying to predict the movement of celestial bodies using mathematics, Brahe was instead focused on making very accurate astronomical measurements, driven by ever improving the observational instruments he used. This allowed for Kepler to test his theoretical ideas against data that he had to collect with the instruments and methods Brahe developed – as he was not allowed to merely copy existent measurement data.

After Kepler and his family got banished for political and religious reasons from Graz, they decided to all move to Prague. For approximately a year, Kepler had a position where he would work for and with Brahe, after which Brahe unexpectedly died. Kepler soon became the Imperial Mathematician of the Holy Roman emperor which allowed him further access to Brahe's catalogue of data. In the years that would follow, Kepler did a lot of research that eventually led to his book *Astronomia Nova* (New Astronomy), published in 1609. He describes the orbit of planet Mars that Brahe and Kepler had thoroughly looked at. This knowledge allowed him to infer that other celestial bodies in the solar system must also show similar behaviour. So it was in this book that Kepler would introduce two of the laws of planetary motion. The third law was later published in 1619, making what we call today '*Kepler's Laws of Planetary Motion*' complete.

Laws (Kepler's laws)**.**

1. **Law of Orbits.** The orbit of every planet is an ellipse with the Sun at one of its foci.

2. **Law of Areas.** The line that connects a planet to the Sun sweeps out equal areas in equal intervals of time.

3. **Law of Periods.** The square of the orbital period of any planet is proportional to the cube of the semi-major axis of its orbit.

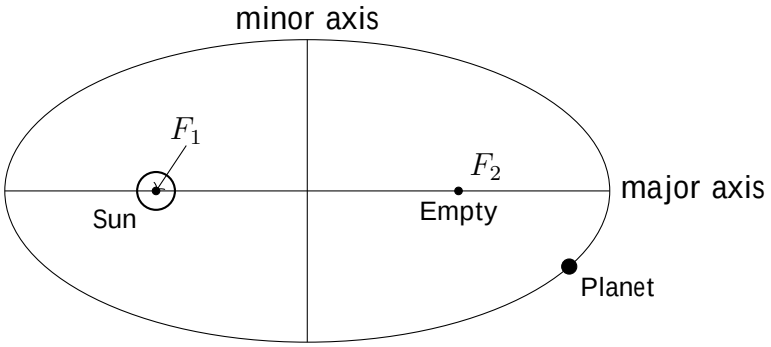

Figure 1.1: An ellipse has a minor and a major axis. On its major axis are two foci: F_1 and F_2. The law of orbits describes that the sun is always at one of these points. The semi-major axis, referred to in the law of periods, is half the length of the major axis, and is the axis from the centre to the perimeter.

1.1 Newton's Laws and the Kepler Problem

What is so remarkable about the laws of Kepler, is that they were comprised only by closely studying the data that Brahe started collecting. One had to wait more than half a century for the theoretical underpinnings to be presented by Isaac Newton (1643–1727) in his book *Philosophiae Naturalis Principia Mathematica* [31]. Newton formulated three laws of motion that described the relations between forces exerted on a body, and the motion of that body. This laid the foundation of the field of classical mechanics.

Laws (Newton's laws)**.**

1. In the absence of a force, a body is at rest or moving at constant velocity in a straight line.

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 the 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 empirical laws by Kepler now had a theoretical basis, and at this point, it could be fully explained why celestial bodies move in an elliptical manner rather than in a circle.

We inform the reader that we make the assumption that a body is described by a point mass, that is, a point in space where all mass of a body is concentrated. More specifically, this point is the centre of mass of the body. We moreover assume that the mass of a body is constant. A body, or, a point mass, with mass m we shall simply refer to as *mass* m.

Newton's influential book, shortly called *Principia*, also included the law of universal gravitation. This law states that every body exerts a force on every other body. In more mathematical terms, the force $\mathbf{F}_{12}$ that a mass m_1,

positioned at $\mathbf{r}_1$, exerts on a mass m_2, positioned at $\mathbf{r}_2$, is given by:

$$\mathbf{F}_{12} = -G\,\frac{m_1 m_2}{r_{12}^2}\,\hat{\mathbf{r}}_{12}, \tag{1.1}$$

where G is the gravitational constant, $\mathbf{r}_{12} = \mathbf{r}_2 - \mathbf{r}_1$ is the vector pointing from m_1 to m_2, r_{12} is the length of $\mathbf{r}_{12}$[(i)], and lastly $\hat{\mathbf{r}}_{12}$ is the unit vector in the direction of $\mathbf{r}_{12}$.

Newton's law of universal gravitation immediately sparks a question. How do we obtain the trajectory of motion of the, in general, n masses when the only force exerted on each body is determined by gravitational force of the other bodies? This is what is regarded as the n-body problem under gravitational force. Unfortunately, it is impossible to solve this problem for $n \geq 3$. However, the case of $n = 2$ is already very much of interest. Consider for example the two-body problem of earth orbiting the sun, or a satellite orbiting earth. Before delving deeper into the two-body problem, we descry that what we arrived at in *Equation* (1.1) exactly follows the form of the Kepler problem.

Kepler problem. The Kepler problem seeks to determine the trajectory of motion of two bodies interacting by a central force $\mathbf{F}$ that is proportional to the inverse square of the distance r between them:

$$\mathbf{F} = \frac{k}{r^2}\,\hat{\mathbf{r}}, \qquad k \text{ constant.} \tag{1.2}$$

where $\hat{\mathbf{r}}$ is the vector connecting the two bodies scaled to unit length.

Besides the gravitational force described by Newton, another force that follows the form of the Kepler problem is the Coulomb force. Imagine two charged particles, with charges q_1 and q_2, located at $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively. Then, the force on q_2 caused by q_1 is the Coulomb force and this is given as follows:

$$\mathbf{F} = \frac{1}{4\pi\varepsilon_0}\,\frac{q_1 q_2}{r_{12}^2}\,\hat{\mathbf{r}}_{12}, \tag{1.3}$$

where ε_0 is the permittivity of free space (constant), and $\mathbf{r}_{12}$ is defined in the same manner as above. To make it clear that the Coulomb force indeed follows the form of the Kepler problem as seen in *Equation* (1.2), let $k = q_1 q_2/(4\pi\varepsilon_0)$, and $\mathbf{r} = \mathbf{r}_{12}$.

1.2 Two- to One-Body Problem

Given an isolated system of two bodies with masses m_1 and m_2 under the influence of a gravitational force, and their positions $\mathbf{r_1}$ and $\mathbf{r_2}$, respectively. The goal is to attain the trajectory of the two bodies. A useful fact is that this problem is equivalent to finding the motion of one body with mass

$$\mu = \frac{m_1 m_2}{m_1 + m_2}, \tag{1.4}$$

[(i)] Throughout the text, we use the notational convention $\|\mathbf{v}\| = v$ for any vector $\mathbf{v}$ with $\|\cdot\|$ denoting the norm.

which is called the reduced mass [1]. That is, the two-body problem can be reduced to a one-body problem.

Using Newton's second and third laws, the equations of motion are given by:

$$m_1\ddot{\mathbf{r}}_1 = \mathbf{F}_{21} \qquad \text{and} \qquad m_2\ddot{\mathbf{r}}_2 = \mathbf{F}_{12} = -\mathbf{F}_{21},$$

where $\ddot{\mathbf{r}} := \mathrm{d}^2\mathbf{r}/\mathrm{d}t^2$. The gravitational force is given by *Equation* (1.1), and therefore

$$m_1\ddot{\mathbf{r}}_1 = -G\,\frac{m_1 m_2}{r_{21}^2}\,\hat{\mathbf{r}}_{21},$$
$$m_2\ddot{\mathbf{r}}_2 = -G\,\frac{m_1 m_2}{r_{12}^2}\,\hat{\mathbf{r}}_{12}.$$

The two moving bodies with masses m_1 and m_2 have a centre of mass that itself is moving through space. The position of the centre of mass is given by the following vector:

$$\mathbf{r}_{\mathsf{CM}} := \underbrace{\frac{m_1}{m_1+m_2}}_{=:c_1}\mathbf{r}_1 + \underbrace{\frac{m_2}{m_1+m_2}}_{=:c_2}\mathbf{r}_2.$$

Note that $c_1, c_2 > 0$ and $c_1 + c_2 = 1$. See *Figure* 1.2 for a schematic outline of the various vectors.

It turns out that $\mathbf{r}_{\mathsf{CM}}$ has zero acceleration, that is, it is moving at a constant velocity.

Claim. $\ddot{\mathbf{r}}_{\mathsf{CM}} = \mathbf{0}$.

Proof. By rewriting $\ddot{\mathbf{r}}_{\mathsf{CM}}$ using Newton's second and third laws, the result is readily obtained:

$$\begin{aligned}
\ddot{\mathbf{r}}_{\mathsf{CM}} = c_1\ddot{\mathbf{r}}_{\mathbf{1}} + c_2\ddot{\mathbf{r}}_{\mathbf{2}} &= c_1\mathbf{a_1} + c_2\mathbf{a_2} \\
&= c_1\frac{\mathbf{F_{21}}}{m_1} + c_2\frac{\mathbf{F_{12}}}{m_2} && 2^{\text{nd}}\text{ law} \\
&= \frac{m_1}{m_1+m_2}\frac{\mathbf{F_{21}}}{m_1} - \frac{m_2}{m_1+m_2}\frac{\mathbf{F_{21}}}{m_2} && 3^{\text{rd}}\text{ law} \\
&= \frac{1}{m_1+m_2}\mathbf{F_{21}} - \frac{1}{m_1+m_2}\mathbf{F_{21}} \\
&\boxed{= \mathbf{0}}.
\end{aligned}$$

□

We note that this is a result of Newton's first law. The forces acting on the bodies are said to be internal to the system of these bodies. Because we are considering an isolated system, there is no way for the system to force itself. This moreover means that there are not outside forces acting on the system, and therefore on the centre of mass. Hence, the there would be no acceleration of the centre of mass.

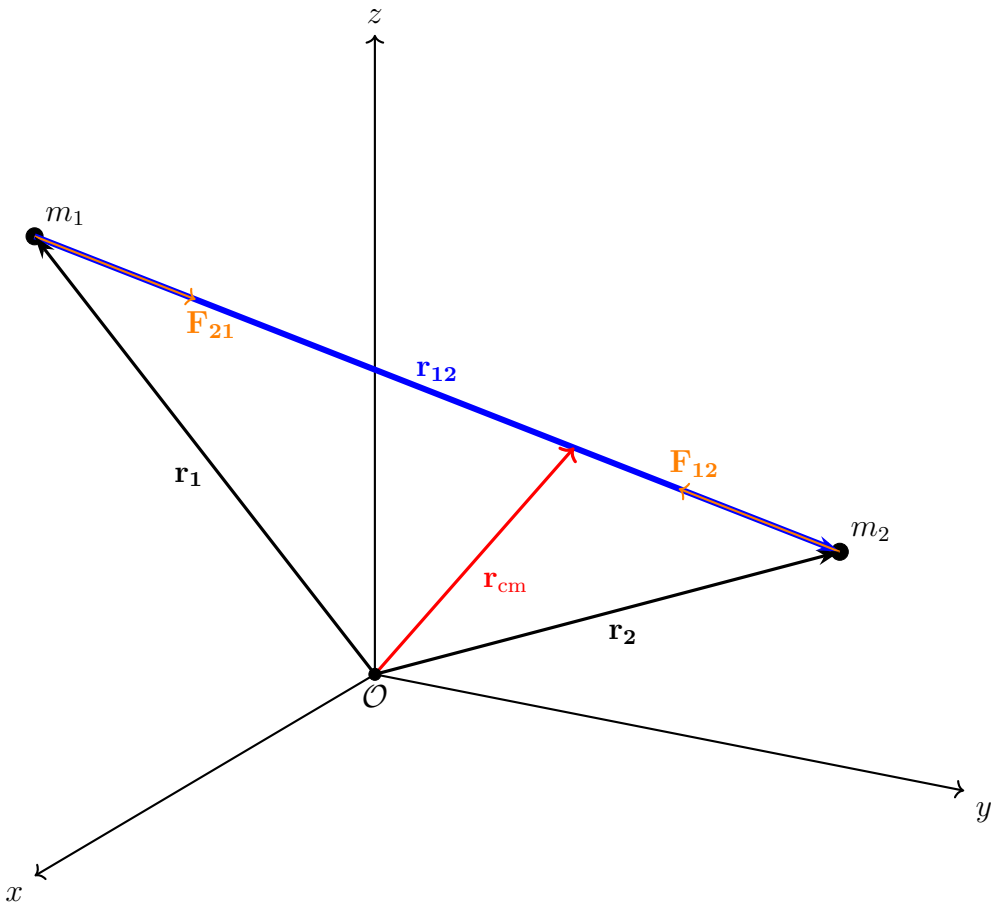

Figure 1.2: The masses m_1 and m_2 are located at $\mathbf{r}_1$ and $\mathbf{r}_2$, respectively. Here, $\mathbf{r}_{\mathsf{CM}}$ is the centre of mass of the two bodies. In this figure we assume $m_2 > m_1$, resulting in $\mathbf{r}_{\mathsf{CM}}$ being closer to the body with mass m_2.

In light of this, it makes sense to switch to an inertial frame of reference that has $\mathbf{r}_{\mathsf{CM}}$ at its origin, i.e. $\mathcal{O}' = \mathbf{r}_{\mathsf{CM}}$.

We then have

$$\mathbf{0} = \mathbf{r}_{\mathsf{CM}} = \frac{m_1}{m_1 + m_2}\mathbf{r_1} + \frac{m_2}{m_1 + m_2}\mathbf{r_2},$$

and multiplying by $m_1 + m_2$ gives

$$m_1\mathbf{r_1} + m_2\mathbf{r_2} = \mathbf{0}. \tag{$*$}$$

On the other hand, notice that the vector between $\mathbf{r_1}$ and $\mathbf{r_2}$ is

$$\mathbf{r_1} - \mathbf{r_2} =: \mathbf{r}. \tag{$**$}$$

(Also see *Figure* 1.3.) Now $\mathbf{r_1}$ and $\mathbf{r_2}$ can be expressed by performing operations on ($*$) and ($**$), and after a careful look it becomes clear that ($*$) $+ m_2$($**$) will

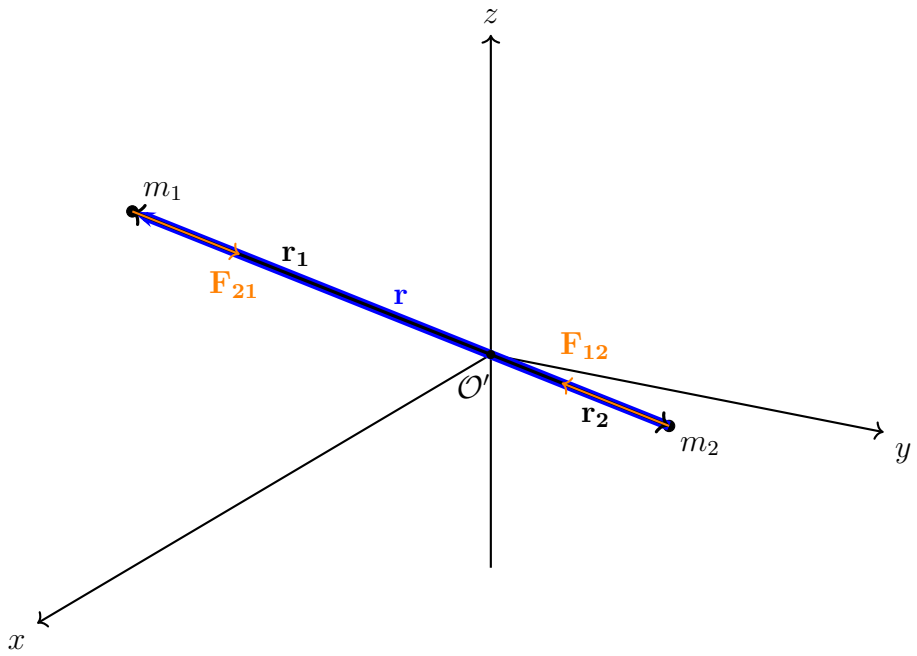

Figure 1.3: New origin $\mathcal{O}'$ at which $\mathbf{r}_{\mathsf{CM}}$ is located.

provide us with an expression of $\mathbf{r_1}$ while $(*) - m_1(**)$ will do so for $\mathbf{r_2}$:

$$\underbrace{m_1\mathbf{r_1} + m_2\mathbf{r_2} + m_2\mathbf{r_1} - m_2\mathbf{r_2}}_{(*)+m_2(**)} = m_2\mathbf{r} \quad \Rightarrow \quad (m_1+m_2)\mathbf{r_1} = m_2\mathbf{r}$$

$$\Rightarrow \quad \boxed{\mathbf{r_1} = \frac{m_2}{m_1+m_2}\mathbf{r}}, \tag{1.5}$$

$$\underbrace{m_1\mathbf{r_1} + m_2\mathbf{r_2} - m_1\mathbf{r_1} + m_1\mathbf{r_2}}_{(*)-m_1(**)} = -m_1\mathbf{r} \quad \Rightarrow \quad (m_1+m_2)\mathbf{r_2} = -m_1\mathbf{r}$$

$$\Rightarrow \quad \boxed{\mathbf{r_2} = -\frac{m_1}{m_1+m_2}\mathbf{r}}. \tag{1.6}$$

These results will prove to be useful later. First we develop some notion of energies.

Definition 1.2.1 (Kinetic and potential energy)**.** Consider a body with mass m and velocity $\mathbf{v}$.

- The **kinetic energy** K of the body is given by $K := \frac{1}{2}mv^2$.
- The **potential energy** V of the body is given such that $-\nabla V = \mathbf{F} = m\dot{\mathbf{v}}$. Here ∇ denotes the gradient.

The kinetic energy is defined relatively straightforward. However, to obtain the potential energy of our system, some e□ort is required.

Claim. Using the relative motion vector $\mathbf{r}$ which connects two bodies, the potential energy $V(\mathbf{r})$ in a gravitational field is given by $V(\mathbf{r}) = -Gm_1m_2/r$.

Proof. We have that $-\nabla V = \mathbf{F}$. The gravitational force $\mathbf{F}$ is given in *Equation* (1.1), and hence, when writing $\mathbf{F}$ in terms of the vector $\mathbf{r}$, we obtain

$$-\nabla V(\mathbf{r}) = \mathbf{F} = -G\frac{m_1 m_2}{r^2}\hat{\mathbf{r}}.$$

Note that $V(\mathbf{r})$ is the work done by an *external agent* 'moving the body from ∞ to $\mathbf{r}$'[(ii)]. Therefore, the work done by the gravitational field is the negative of the work done by the external agent. Hence,

$$V(\mathbf{r}) = -\int_{\mathbf{r}}^{\infty} -\mathbf{F}\cdot \mathrm{d}\mathbf{r}.$$

(Notice that $\mathbf{F}$ is pointing radially inward.) Consider the parametrisation $C = \{\mathbf{R}(u) \mid \mathbf{R}(u) = u\mathbf{r}, 1 \leq u < \infty\}$. Then we find

$$\begin{aligned}
V(\mathbf{r}) &= -\int_C -\mathbf{F}\cdot \mathrm{d}\mathbf{R} \\
&= -\int_1^{\infty} G\frac{m_1 m_2}{R^2}\hat{\mathbf{R}}\cdot\mathbf{r}\,\mathrm{d}u && \text{since } \mathrm{d}\mathbf{R} = \mathbf{r}\,\mathrm{d}u \\
&= -\int_1^{\infty} G\frac{m_1 m_2}{u^2 r^2}\frac{u}{ur}\mathbf{r}\cdot\mathbf{r}\,\mathrm{d}u && \text{since } R(u) = ur \\
&= -G\frac{m_1 m_2}{r}\lim_{x\to\infty}\int_1^x \frac{1}{u^2}\,\mathrm{d}u && \text{since } \mathbf{r}\cdot\mathbf{r} = r^2 \\
&= -G\frac{m_1 m_2}{r}\lim_{x\to\infty}\left[-\frac{1}{u}\right]_{u=1}^{x} \\
&= -G\frac{m_1 m_2}{r},
\end{aligned}$$

as desired. □

It is customary to define the constant $k := Gm_1 m_2$, also known as the gravitational coupling constant. The potential energy can then be compactly written as $V(\mathbf{r}) = -k/r$.

Often one wants to consider the total energy of a system (that is, total kinetic *plus* potential energy). The Hamiltonian function allows us to do so, and is defined below. We will see that this is the final key element in reducing to a one-body system.

Definition 1.2.2 (Hamiltonian)**.** Consider the gravitational two-body problem with reduced mass μ and position vector $\mathbf{r}$. The **Hamiltonian** H is a function that represents the total energy of the system. It is given by

$$\begin{aligned}
H : \mathbb{R}^3 \setminus \{\mathbf{0}\} \times \mathbb{R}^3 &\to \mathbb{R} \\
(\mathbf{r}, \mathbf{p}) &\mapsto K + V = \frac{p^2}{2\mu} - \frac{k}{r},
\end{aligned}$$

[(ii)] We let the external agent move the body from ∞ since $V(\mathbf{r}) \to 0$ as $r \to \infty$, thereby simplifying the expression we end up with. For additional information, we refer to [34].

where $\mathbf{p} := m\mathbf{v}$ is the *linear momentum*, and k is the gravitational coupling constant.

The Hamiltonian H in our system is given by

$$\begin{aligned} H = K + V &= \frac{1}{2}m_1\dot{r}_1^2 + \frac{1}{2}m_2\dot{r}_2^2 + V(\mathbf{r}) \\ &= \frac{1}{2}\left(m_1 v_1^2 + m_2 v_2^2\right) - \frac{k}{r}. \end{aligned}$$

By *Equations* (1.5) and (1.6), $v_1 = \dot{r}_1 = \dfrac{m_2}{m_1+m_2}\dot{r} = \dfrac{m_2}{m_1+m_2}v$ and $v_2 = \dot{r}_2 = \dfrac{m_1}{m_1+m_2}\dot{r} = \dfrac{m_1}{m_1+m_2}v$. Substituting in the above gives

$$\begin{aligned} H &= \frac{1}{2}\left(m_1\frac{m_2^2}{(m_1+m_2)^2}v^2 + m_2\frac{m_1^2}{(m_1+m_2)^2}v^2\right) - \frac{k}{r} \\ &= \frac{1}{2}\underbrace{\frac{m_1 m_2}{m_1+m_2}}_{=\mu}v^2 - \frac{k}{r} \\ &\boxed{= \frac{1}{2}\mu v^2 - \frac{k}{r}}. \end{aligned}$$

Notice the introduction of the reduced mass μ. Moreover, v and r are derived from $\mathbf{r}$ (the relative motion vector). So it becomes clear from the Hamiltonian that the two-body problem has successfully been reduced to a one-body problem, where the hypothetical single body is considered to have 'mass' μ and 'position' $\mathbf{r}$.

At this point, another important observation to make here is that $\dot{H} = 0$. This means that the total energy in our system is conserved. So any changes in energy must be accounted for by transfers between the different forms of energy within the system.

Claim (Conservation of energy)**.** The total energy of the isolated two-body problem (or equivalent one-body problem) is constant with time.

Proof. First of all, the equations of motion in terms of position $\mathbf{r}(t)$ and linear momentum $\mathbf{p}(t)$, where t denotes time, can be expressed via the following ordinary differential equations:

$$\begin{cases} \mu\dot{\mathbf{r}}(t) = \mathbf{p}(t) \\ \dot{\mathbf{p}}(t) = \mathbf{F}\big(\mathbf{r}(t)\big), \end{cases} \tag{1.7}$$

with some initial position $\mathbf{r}(0) = \mathbf{r}_0$ and momentum $\mathbf{p}(0) = \mathbf{p}_0$. On the other hand, using the dot product $(\cdot)$, the Hamiltonian can be written as

$$H\left(\mathbf{r}(t), \mathbf{p}(t)\right) = \frac{1}{2\mu}\mathbf{p}(t)\cdot\mathbf{p}(t) - \frac{k}{r(t)},$$

and so $\dot{H}$ is given by

$$\begin{aligned}\dot{H}\big(\mathbf{r}(t),\mathbf{p}(t)\big) &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\frac{1}{2\mu}\mathbf{p}(t)\cdot\mathbf{p}(t) - \frac{k}{r(t)}\right)\\ &= \frac{1}{2\mu}\big(\dot{\mathbf{p}}(t)\cdot\mathbf{p}(t) + \mathbf{p}(t)\cdot\dot{\mathbf{p}}(t)\big) - k\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{r(t)}\\ &= \frac{1}{\mu}\big(\mathbf{p}(t)\cdot\dot{\mathbf{p}}(t)\big) - k\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{r(t)}.\end{aligned}$$

Substituting the equations of motion into the above gives

$$\begin{aligned}\dot{H}\big(\mathbf{r}(t),\mathbf{p}(t)\big) &= \frac{1}{\mu}\left[\big(\mu\dot{\mathbf{r}}(t)\big)\cdot\mathbf{F}\big(\mathbf{r}(t)\big)\right] - k\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{r(t)}\\ &= \dot{\mathbf{r}}(t)\cdot\left[-\nabla V\big(\mathbf{r}(t)\big)\right] - k\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{r(t)} && \text{since } \mathbf{F} = -\nabla V\\ &= -\frac{\mathrm{d}}{\mathrm{d}t}V\big(\mathbf{r}(t)\big) - k\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{r(t)} && \text{by the chain rule}\\ &= k\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{r(t)} - k\frac{\mathrm{d}}{\mathrm{d}t}\frac{1}{r(t)} && \text{since } V(\mathbf{r}) = -\frac{k}{r}\\ &\boxed{= 0}.\end{aligned}$$

So, $\dot{H}\big(\mathbf{r}(t),\mathbf{p}(t)\big) = 0$ meaning that the Hamiltonian function along solutions $\mathbf{r}(t)$ and $\mathbf{p}(t)$ of *Equation* (1.7) is constant. This in turn means that the total energy within of the isolated system is conserved. □

1.3 Kepler's Laws Revisited: Elementary Proofs

In this section, we use the developed theoretical framework to obtain Kepler's empirical second law:

'*The line that connects a planet to the Sun sweeps out equal areas in equal intervals of time.*'

Let $\mathbf{r}(t)$ be the position of a planet at time t. As illustrated in *Figure* 1.5, in a particular time interval $(t, t+\Delta t)$, the vector $\mathbf{r}(t)$ sweeps out a triangle of area

$$\Delta A = \frac{1}{2}\left|\mathbf{r}(t)\times\Delta\mathbf{r}(t)\right|,$$

where $\Delta\mathbf{r}(t) := \mathbf{r}(t+\Delta t) - \mathbf{r}(t)$, i.e. the vector from $\mathbf{r}(t)$ to $\mathbf{r}(t+\Delta t)$. The rate of change in area is then

$$\frac{\Delta A}{\Delta t} = \frac{1}{2}\frac{|\mathbf{r}\times\Delta\mathbf{r}|}{\Delta t}.$$

This can be carefully rewritten by using how $\Delta\mathbf{r}(t)$ is defined, to obtain

$$\frac{\Delta A}{\Delta t} = \frac{1}{2}\left|\mathbf{r}(t)\times\frac{\mathbf{r}(t+\Delta t)-\mathbf{r}(t)}{\Delta t}\right|.$$

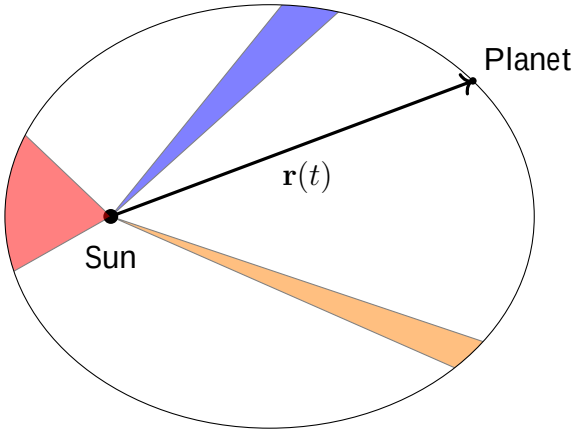

Figure 1.4: Illustration of Kepler's second law. All coloured areas, which were swept out in an equal time interval, are equal in area. Taken and amended from [41].

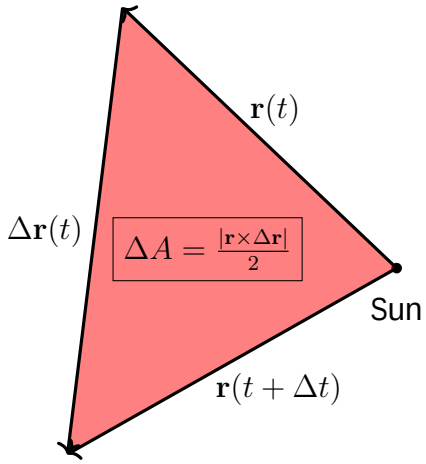

Figure 1.5: An area on the left, such as the red one, can be approximated by a triangle since the time intervals will be taken to be infinitesimally small.

By letting $\Delta t \to 0$ derivatives are introduced, that is

$$\begin{aligned}\frac{\Delta A}{\Delta t} \quad \xrightarrow{\Delta t\to 0} \quad \frac{\mathrm{d}A}{\mathrm{d}t} &= \frac{1}{2}\left|\mathbf{r}(t)\times\dot{\mathbf{r}}(t)\right| \\ &= \frac{1}{2\mu}\left|\mathbf{r}(t)\times\mu\mathbf{v}(t)\right| \\ &= \frac{1}{2\mu}\left|\mathbf{r}(t)\times\mathbf{p}(t)\right|.\end{aligned}$$

The vector $\mathbf{r}(t)\times\mathbf{p}(t)$ present in the expression we end up with, is called the *angular momentum* and is denoted by $\mathbf{L}(\mathbf{r},\mathbf{p})$. In successfully proving Kepler's second law, it remains to show that $\left|\mathbf{L}\big(\mathbf{r}(t),\mathbf{p}(t)\big)\right|$ is constant, as then $\mathrm{d}A/\mathrm{d}t$ is also constant, implying the swept out area A is changing in time in a constant manner. In fact, we will prove something stronger, namely that $\mathbf{L}\big(\mathbf{r}(t),\mathbf{p}(t)\big)$ is constant (and not just its length).

Claim (Conservation of angular momentum)**.** The angular momentum of the isolated two-body problem (or equivalent one-body problem) is constant with time.

Proof. Consider again the equations of motion in terms of position $\mathbf{r}(t)$ and linear momentum $\mathbf{p}(t)$, with t denoting time:

$$\begin{cases} \mu\dot{\mathbf{r}}(t) = \mathbf{p}(t) \\ \dot{\mathbf{p}}(t) = \mathbf{F}\big(\mathbf{r}(t)\big). \end{cases} \tag{1.8}$$

For completeness, let the initial values be $\mathbf{r}(0) = \mathbf{r}_0$ and $\mathbf{p}(0) = \mathbf{p}_0$, with $\mathbf{r}_0$ some initial position of the body, and $\mathbf{p}_0$ its initial linear momentum. Now, using these equations of motion, the angular momentum can be written as

$$\begin{aligned} \dot{\mathbf{L}}\big(\mathbf{r}(t), \mathbf{p}(t)\big) &= \frac{\mathrm{d}}{\mathrm{d}t}\big(\mathbf{r}(t) \times \mathbf{p}(t)\big) \\ &= \dot{\mathbf{r}}(t) \times \mathbf{p}(t) + \mathbf{r}(t) \times \dot{\mathbf{p}}(t) \\ &= \frac{1}{\mu}\mathbf{p}(t) \times \mathbf{p}(t) + \mathbf{r}(t) \times \mathbf{F}\big(\mathbf{r}(t)\big). \end{aligned}$$

Since the cross product of a vector with itself is zero, the first term disappears. For the second term, note that the force is given by $\mathbf{F}(\mathbf{r}) = -(k/r^2)\hat{\mathbf{r}} = -(k/r^3)\mathbf{r}$. Therefore,

$$\begin{aligned} \dot{\mathbf{L}}\big(\mathbf{r}(t), \mathbf{p}(t)\big) &= \mathbf{r}(t) \times \frac{-k}{\big(r(t)\big)^3}\mathbf{r}(t) \\ &\boxed{= \mathbf{0}}, \end{aligned}$$

so this term disappears as well because of a vector being crossed with itself. It is concluded that $\dot{\mathbf{L}}\big(\mathbf{r}(t), \mathbf{p}(t)\big) = 0$, i.e. the angular momentum along solutions $\mathbf{r}(t)$ and $\mathbf{p}(t)$ is constant. So, angular momentum of the isolated system is conserved. □

This also concludes the proof of Kepler's second law, as

$$\frac{\mathrm{d}A}{\mathrm{d}t} = \frac{1}{2\mu}\left|\mathbf{r}(t) \times \mathbf{p}(t)\right| = \frac{1}{2\mu}\underbrace{\left|\mathbf{L}\big(\mathbf{r}(t), \mathbf{p}(t)\big)\right|}_{\text{constant}},$$

i.e. $\mathrm{d}A/\mathrm{d}t$ is constant. The remarkable observation one can make here is that the conservation of angular momentum implies Kepler's second law.

For Kepler's first law, a similar observation can be made. Recall that this law states:

'*The orbit of every planet is an ellipse with the Sun at one of its foci.*'

It turns out that this law is implied by the conservation of two objects, namely: energy, and a special vector $\mathbf{A}$. This of course needs some explaining, as will be done below. For this, we follow the thought of [21], which we refer to for a more complete treatment, as below we consider only the most crucial aspects.

Moreover, this reference includes alternative ways of proving the same idea. We have seen before the conservation of energy, so lets turn our attention towards this yet mysterious vector $\mathbf{A}$, and why it is a conserved object.

Definition 1.3.1 (Laplace-Runge-Lenz vector)**.** Consider a body with mass μ and position $\mathbf{r}$ under the influence of a force of the form $\mathbf{F} = -(k/r^2)\hat{\mathbf{r}}$. Then the **Laplace-Runge-Lenz vector** is defined by

$$\mathbf{A} = \mathbf{p} \times \mathbf{L} - k\mu\hat{\mathbf{r}},$$

where $\mathbf{p} = \mu\dot{\mathbf{r}}$ is the linear momentum, and $\mathbf{L} = \mathbf{r} \times \mathbf{p}$ is the angular momentum.

As mentioned, the vector $\mathbf{A}$ is conserved, which can be directly shown using the definition.

Theorem 1.3.2. The Laplace-Runge-Lenz (LRL) vector $\mathbf{A}$ is conserved.

Proof. The LRL vector is given by

$$\mathbf{A} = \mathbf{p}(t) \times \mathbf{L}(t) - \frac{k\mu}{r(t)}\,\mathbf{r}(t),$$

with $\mathbf{p}(t)$ and $\mathbf{r}(t)$ being solutions of the equations of motions, see *Equation* (1.8). Hence its derivative is

$$\begin{aligned}\dot{\mathbf{A}} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\mathbf{p}(t) \times \mathbf{L}(t) - \frac{k\mu}{r(t)}\,\mathbf{r}(t)\right) \\ &= \dot{\mathbf{p}}(t) \times \mathbf{L}(t) + \mathbf{p}(t) \times \dot{\mathbf{L}}(t) - k\mu\frac{\mathrm{d}}{\mathrm{d}t}\frac{\mathbf{r}(t)}{r(t)}.\end{aligned}$$

It was seen that $\dot{\mathbf{L}} = 0$, and therefore the second term disappears. Of interest is the term $\dot{\mathbf{p}} \times \mathbf{L}$, which can be rewritten by using how $\mathbf{p}$ and $\mathbf{L}$ are defined, and thereafter using the rule

$$\mathbf{u} \times (\mathbf{v} \times \mathbf{w}) = (\mathbf{u} \cdot \mathbf{w})\mathbf{v} - (\mathbf{u} \cdot \mathbf{v})\mathbf{w}$$

for vectors $\mathbf{u}, \mathbf{v}, \mathbf{w} \in \mathbb{R}^3$, see [21, *Chapter* 2]. So:

$$\begin{aligned}\dot{\mathbf{p}}(t) \times \mathbf{L}(t) &= \mu\mathbf{a}(t) \times \big(\mathbf{r}(t) \times \mathbf{p}(t)\big) \\ &= \mathbf{F}\big(\mathbf{r}(t)\big) \times \big(\mathbf{r}(t) \times \mu\mathbf{v}(t)\big) \\ &= -\frac{k\mu}{r^3}\big[\mathbf{r}(t) \times \big(\mathbf{r}(t) \times \dot{\mathbf{r}}(t)\big)\big] \\ &= -\frac{k\mu}{r^3}\big[\big(\mathbf{r}(t) \cdot \dot{\mathbf{r}}(t)\big)\mathbf{r}(t) - \big(\mathbf{r}(t) \cdot \mathbf{r}(t)\big)\dot{\mathbf{r}}(t)\big].\end{aligned}$$

Now, $\mathbf{r} \cdot \mathbf{r} = r^2$ and

$$\mathbf{r} \cdot \dot{\mathbf{r}} = \frac{\dot{\mathbf{r}} \cdot \mathbf{r} + \mathbf{r} \cdot \dot{\mathbf{r}}}{2} = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}\big(\mathbf{r} \cdot \mathbf{r}\big) = \frac{1}{2}\frac{\mathrm{d}}{\mathrm{d}t}r^2 = r\dot{r},$$

so the above becomes

$$\begin{aligned}\dot{\mathbf{p}}(t) \times \mathbf{L}(t) &= -\frac{k\mu}{r^3}\left[r(t)\dot{r}(t)\mathbf{r}(t) - \big(r(t)\big)^2\dot{\mathbf{r}}(t)\right] \\ &= k\mu\left(-\frac{\dot{r}(t)}{\big(r(t)\big)^2}\mathbf{r}(t) - \frac{1}{r(t)}\dot{\mathbf{r}}(\mathbf{t})\right) \\ &= k\mu\frac{\mathrm{d}}{\mathrm{d}t}\frac{\mathbf{r}(t)}{r(t)}.\end{aligned}$$

The desired result quickly follows:

$$\begin{aligned}\dot{\mathbf{A}} &= \dot{\mathbf{p}}(t) \times \mathbf{L}(t) - k\mu\frac{\mathrm{d}}{\mathrm{d}t}\frac{\mathbf{r}(t)}{r(t)} \\ &= k\mu\frac{\mathrm{d}}{\mathrm{d}t}\frac{\mathbf{r}(t)}{r(t)} - k\mu\frac{\mathrm{d}}{\mathrm{d}t}\frac{\mathbf{r}(t)}{r(t)} \\ &\boxed{= \mathbf{0}}.\end{aligned}$$

Therefore, the LRL vector is constant along solutions $\mathbf{r}(t)$ and $\mathbf{p}(t)$, implying the conservation of that vector. □

The question that still lingers is how the Laplace-Runge-Lenz vector plays a role in Kepler's first law. Indeed, this is not directly obvious, but what we can do is carefully looking at the geometry of a planet moving around the Sun. Suppose that the Sun is conveniently located at the origin, and consider again the Hamiltonian $H = K + V = p^2/(2\mu) - k/r$. In the case where the planet is orbiting the Sun, we must have that $K < -V$ i.e. $H < 0$, otherwise the potential energy would be too weak to hold the planet in orbit. (Note that $K \geq 0$, and H remains constant by the conservation of energy.) This translates to the idea that $V(\mathbf{r}) \leq H < 0$, so $-k/r \leq H$ and hence $r \leq -k/H$. The planet is therefore said to be bounded inside a sphere $\mathcal{S}$ centred at the origin with radius $-k/H$ [21].

Notice that the angular momentum is given by $\mathbf{L} = \mathbf{r} \times \mathbf{p}$, so $\mathbf{L}$ is perpendicular to the plane in which $\mathbf{r}$ and $\mathbf{p}$ are situated. Therefore, the earlier reasoning can be easily visualised by considering the plane perpendicular to $\mathbf{L}$, see *Figure* 1.6, on which we have a circle $\mathcal{C}$ representing the cross section of the sphere $\mathcal{S}$ on that plane (so $\mathcal{C}$ has radius $-k/H$ and is centred at the origin). What is now of importance is that the circle $\mathcal{C}$ is the boundary of the disk where the planet has energy $H < 0$.

The planet is in orbit, the latter we shall name $\mathcal{E}$, and has position $\mathbf{r}$ and linear momentum $\mathbf{p}$. The tangent line of the planet in $\mathcal{E}$ at $\mathbf{r}$ moving with velocity $\mathbf{v}$, we define as $\mathcal{L}$. Clearly, this line is parallel to $\mathbf{p}$. We moreover consider a vector $\mathbf{s}$ which is the projection of $\mathbf{r}$ from the origin to $\mathcal{C}$. By reflecting $\mathbf{s}$ orthogonally in the line $\mathcal{L}$, we obtain the point $\mathbf{t}$. Already by looking at *Figure* 1.6 one could hypothesize that $\mathbf{t}$ is at the point which we previously called 'the empty focus point of the orbit'. This turns out to be true, and follows from how this point is related to what we have seen before.

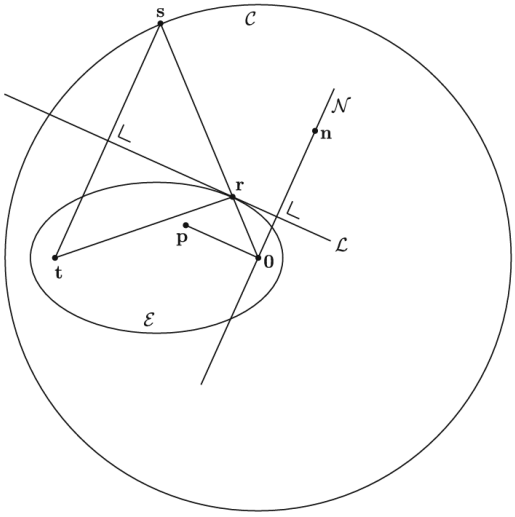

Figure 1.6: The plane perpendicular to $\mathbf{L}$. Taken from [21].

Theorem 1.3.3. Let the vector $\mathbf{t}$ be as constructed above. The following two hold:

1. The vector $\mathbf{t}$ can be written as
$$\mathbf{t} = \frac{1}{\mu H}\mathbf{A}.$$
2. The vector $\mathbf{t}$ is conserved.

Proof. For (1), see [21] for a concise geometrical proof. On the other hand, (2) easily follows from (1). As both H and $\mathbf{A}$ are conserved i.e., $\dot{H} = 0$ and $\dot{\mathbf{A}} = \mathbf{0}$, we must have $\dot{\mathbf{t}} = \mathbf{0}$. That is to say $\mathbf{t}$ is indeed conserved. □

Corollary 1.3.4. The orbit $\mathcal{E}$ is an ellipse with foci $\mathbf{0}$ and $\mathbf{t}$, and major axis of length $-k/H$.

Proof. Consider *Figure* 1.6. We are concerned with $|\mathbf{t} - \mathbf{r}|$ and $|\mathbf{r} - \mathbf{0}|$. Since $\mathbf{t}$ is the orthogonal reflection of $\mathbf{s}$ in $\mathcal{L}$, we have $|\mathbf{t} - \mathbf{r}| = |\mathbf{s} - \mathbf{r}|$. So:

$$\begin{aligned} |\mathbf{t} - \mathbf{r}| + |\mathbf{r} - \mathbf{0}| &= |\mathbf{s} - \mathbf{r}| + |\mathbf{r} - \mathbf{0}| \\ &= |\mathbf{s} - \mathbf{0}| \\ &= s. \end{aligned}$$

Here, s is just the radius of $\mathcal{C}$, so $s = -k/H$. Therefore it is concluded that $\mathcal{E}$ is an ellipse with foci $\mathbf{0}$ and $\mathbf{t}$, and major axis of length $-k/H$. □

This now proves Kepler's first law, that the orbit of a planet is an ellipse with the Sun at one of its foci. We further gathered that at the other foci we have the point $\mathbf{t}$. Analogously to the fact that conservation of angular momentum implies Kepler's second law, we have now also seen that the conservation of energy *and* of the Laplace-Runge-Lenz vector together imply Kepler's first law.

Throughout this chapter, we obtained seven conserved quantities. Namely, H is conserved (+1), $\mathbf{L}$ is conserved (+3), and $\mathbf{A}$ is conserved (+3). However, there are the following constraints on $\mathbf{A}$ [14]:

$$\mathbf{A} \cdot \mathbf{L} = 0 \qquad \text{and} \qquad A^2 = \mu^2 k^2 + 2\mu H L^2.$$

From the first constraints, it follows that the Laplace-Runge-Lenz vector $\mathbf{A}$ is perpendicular to $\mathbf{L}$. This means that once L_x, L_y, and L_z are given, the plane of motion can be determined. Therefore, one only needs two components of $\mathbf{A}$. The second constraint further reduces the amount of components of $\mathbf{A}$ needed to just one. The bottom line is now that, although there are seven conserved quantities, only five of them are independent. Yet this ought to be admired as this actually is the highest amount of conserved quantities possible [19].

1.4 A First Look at (Hidden) Symmetry

We elaborate on the conserved quantities that were found in the previous subsection. As it turns out, they show a tight relationship with what is called *symmetry*. This is an idea we shall look at in a slightly informal manner for now by laying out in bird's eye perspective the essence of the connection between symmetries and conserved quantities within the classical mechanical framework. First of all, let D be some property of a (physical) system that itself is dependent on different quantities $X, Y, Z, \ldots$. For example, the dynamics described by the equations of motion is a possible property. We write $D = D(X, Y, Z, \ldots)$. Now consider some transformation

$$\begin{aligned} X &\to X' \\ Y &\to Y' \\ Z &\to Z' \\ \vdots &\to \vdots. \end{aligned}$$

If we have

$$D(X', Y', Z', \ldots) = D(X, Y, Z, \ldots),$$

then we call D invariant under the transformation. We can now define what the concept of symmetry entails.

Definition 1.4.1 (Symmetry)**.** Invariance under a transformation or class of transformations is referred to as **symmetry**.

Some examples of transformations include spatial and temporal translations, and rotations. We make the following claim.

Claim. The equations of motion of the isolated two-body problem (or equivalent one-body problem) are invariant under (i) time translation and (ii) three-dimensional rotations.

Proof. The equations of motion in terms of position $\mathbf{r}(t)$ and linear momentum $\mathbf{p}(t)$ are

$$\begin{cases} \mu\dot{\mathbf{r}}(t) = \mathbf{p}(t) \\ \dot{\mathbf{p}}(t) = \mathbf{F}\big(\mathbf{r}(t)\big), \end{cases}$$

where t denotes time. The initial position and momentum we consider to be $\mathbf{r}(0) = \mathbf{r}_0$ and $\mathbf{p}(0) = \mathbf{p}_0$, respectively.

(i) Let $t \to t + t_0 =: \tau$ be some time translation, where $t_0 \in \mathbb{R}$ is some constant. Let $\tilde{\mathbf{r}}(t) := \mathbf{r}(\tau)$ and $\tilde{\mathbf{p}}(t) := \mathbf{p}(\tau)$, then

$$\begin{aligned} \dot{\tilde{\mathbf{r}}}(t) &= \dot{\mathbf{r}}(t + t_0) \\ &= \frac{\mathrm{d}(t + t_0)}{\mathrm{d}t} \frac{\mathrm{d}\mathbf{r}(t + t_0)}{\mathrm{d}\tau} \\ &= \frac{\mathrm{d}\mathbf{r}(\tau)}{\mathrm{d}\tau} \\ &= \frac{1}{\mu}\tilde{\mathbf{p}}(t), \end{aligned}$$

hence $\mu\dot{\tilde{\mathbf{r}}}(t) = \tilde{\mathbf{p}}(t)$. In a completely analogous way, one finds $\dot{\tilde{\mathbf{p}}}(t) = \mathbf{F}\big(\mathbf{r}(\tau)\big) = \mathbf{F}\big(\tilde{\mathbf{r}}(t)\big)$. Therefore upon time translation, only the naming of the variables change, not the equations of motion themself. That is, the latter is invariant under time translation.

(ii) Now let $\mathbf{r}(t) \to R\mathbf{r}(t) =: \tilde{\mathbf{r}}(t)$ be some three-dimensional rotational transformation, where R is a matrix representing the respective rotation. We then have

$$\begin{aligned} \dot{\tilde{\mathbf{r}}}(t) &= \frac{\mathrm{d}}{\mathrm{d}t} R\mathbf{r}(t) \\ &= \mathbf{r}(t)\dot{R} + R\dot{\mathbf{r}}(t) \\ &= R\dot{\mathbf{r}}(t) \\ &= \frac{1}{\mu} R\mathbf{p}(t), \end{aligned}$$

and hence if we let $\tilde{\mathbf{p}}(t) := R\mathbf{p}(t)$, then $\mu\dot{\tilde{\mathbf{r}}}(t) = \tilde{\mathbf{p}}(t)$. On the other hand, we have $\dot{\tilde{\mathbf{p}}}(t) = \mathbf{F}\big(\tilde{\mathbf{r}}(t)\big)$. We draw the conclusion that only the naming of variables change, implying invariance of the equations of motion under three-dimensional rotations.

Overall, the equations of motions are invariant under both time translations and three-dimensional rotations. □

We can say, by the claim above, that the Kepler problem has temporal translational symmetry, and three-dimensional rotational symmetry. The former implies that one could look at a body in orbit today and at any later time, and the motion by which that *same* orbit is described is not altered. The latter then, in a similar way, means that we can rotate the orbit of a body and it will not have an e□ect on the dynamics of the system itself. As we shall see shortly,

it turns out that the Kepler problem has even more symmetry than what is already established. In a sense, this additional symmetry is non-obvious as it is not directly clear why it is existent and how it should be thought of. It is for that reason we call it *hidden symmetry*. To see how (hidden) symmetry is related to conserved quantities consider the following non-technical statement[(iii)] [45]:

> '*If a system has a continuous symmetry property, then there are corresponding conserved quantities.*'

Two remarks are at place here. First, we assume all symmetries that are discussed to be continuous[(iv)]. An example of discrete symmetry is where the underlying transformation is temporal or spatial reflection. Moreover, a square is not said to be invariant under any rotation, only rotations by an angle of a multiple of 90 degrees. So a square does not posses continuous rotational symmetry. However, a circle does.

Another remark is that symmetry of an isolated system cannot decrease as the system evolves with time [45, 23].

One could ask if the converse of the statement also holds. It turns out that this is generally not the case. There are conservation conditions that cannot correspond to any symmetry property [19]. However in our case, we can relate all conservations we have seen to symmetries. The conserved quantities were the Hamiltonian H, angular momentum $\mathbf{L}$, and Laplace-Runge-Lenz vector $\mathbf{A}$. The claim above already showed time translational and three-dimensional rotational symmetry. The corresponding conserved quantities turn out to be the Hamiltonian H and angular momentum $\mathbf{L}$, respectively. As was previously mentioned, there is also hidden symmetry at play in the Kepler problem. More specifically, we have four-dimensional rotational symmetry where the corresponding conserved quantities are the Laplace-Runge-Lenz vector together with the angular momentum[(v)]. In *Table* 1.1 we present a complete overview of conserved quantities and symmetries.

Conserved quantity	**Continuous symmetry**
Hamiltonian H	Temporal translation
Angular momentum $\mathbf{L}$	Three-dimensional rotation
Laplace-Runge-Lenz vector $\mathbf{A}$ *and* angular momentum $\mathbf{L}$	Four-dimensional rotation

Table 1.1: The correspondence between conserved quantities and (continuous) symmetries [45]. For example, time translational symmetry implies the existence of a conserved quantity, which turns out to be the Hamiltonian H.

[(iii)] A more sophisticated statement (Noether's theorem) requires Lagrangian or Hamiltonian formalism. See [19, 38] for a Lagrangian treatment of Noether's theorem. On the other hand, [40] discusses how the Hamiltonian framework, where the Hamiltonian is the central object, enables for describing the same theorem.

[(iv)] Continuous symmetries fall within the framework of Lie groups and Lie algebras. We will see this in *Section* 3.3.

[(v)] It is necessary to have six conserved quantities since the rotations in four dimensions form a group, which has *six* generators.

It is not directly clear how symmetry of the Kepler problem in four-dimensional rotations should be interpreted. We provide two ways of interpretation.

1. When applying the respective transformation, a four-dimensional rotation, one finds invariance under three-dimensional rotations of the ellipse that a body is orbiting in. This is similar to the symmetry corresponding to the conservation of solely angular momentum. But moreover, an invariance under changes in the eccentricity, denoted e, is also present. This is a value describing how flat the ellipse is, where $0 \leq e \leq 1$[vi]. If $e = 0$, the ellipse coincides with a circle, and if $e = 1$, it becomes a line. So, varying e corresponds to 'compression' and 'expansion' of the ellipse. Also see *Figure* 1.7.

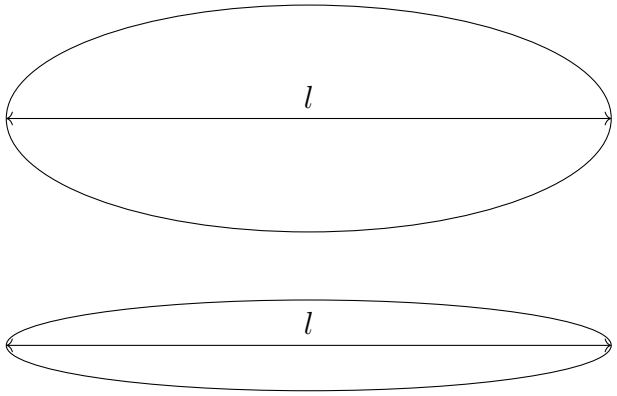

Figure 1.7: Ellipses with different eccentricities.

Recall that the Laplace-Runge-Lenz vector is given by

$$\mathbf{A} = \mathbf{p} \times \mathbf{L} - k\mu\hat{\mathbf{r}},$$

cf. *Definition* 1.3.1. The eccentricity of the relevant ellipse is then

$$e = \frac{A}{|k\mu|}. \tag{1.9}$$

So it is seen that the eccentricity is closely related to $\mathbf{A}$[vii]. The bottom line is that a four-dimensional transformation applied to the Kepler problem rotates the ellipse of orbit, but also affects its shape.

[vi] Recall that we are restricting to bound states only.

[vii] One might object here by saying that since the LRL vector $\mathbf{A}$ is a conserved quantity, surely e must be fixed. So how can the eccentricity change? Indeed, given some system of an isolated two-body problem, $\mathbf{A}$ is conserved and hence e is constant. However, as we apply the four-dimensional transformation to the system, the LRL vector need not be the same as before (note that the angular momentum $\mathbf{L}$ can now also differ). To that end, we call the LRL vector after the transformation $\tilde{\mathbf{A}}$. But by *Equation* (1.9), the eccentricity is now also altered (since k is constant, and we assumed masses are also constant), so we call it $\tilde{e}$. Assuming nothing else happens within the system after the transformation, $\tilde{\mathbf{A}}$ will not change, it is after all a conserved quantity, so neither will the eccentricity $\tilde{e}$.

The idea is that even though the LRL vector is a conserved quantity, this does not mean it is invariant under transformations. Rather, it are the equations of motion that are said to be invariant under (specific) transformations.

2. The *phase space* of a system is the space of all possible states. Here, by state we mean the position *and* momentum of the objects in the system. One can also look only at position, which yields the *configuration space*, and similarly, only at momentum, which yields the *momentum space*[(viii)] [44]. While the conservation of angular momentum has a symmetry that only requires consideration of configuration space, one needs to consider phase space when we add the conservation of the Laplace-Runge-Lenz vector. We can view the four-dimensional rotation transformation as a rotation in phase space.

In the chapters that follow, we also look at the (hidden) symmetry of the Kepler problem, but in a quantum mechanical framework.

[(viii)] In general, the configuration space can be described by some manifold M. Then, momentum space is in turn the cotangent space of M. For more details, we refer to [27, 46].

Chapter 2

The Quantum Kepler Problem

Up till here, we studied the Kepler problem and its symmetries in classical mechanics. The aim of this chapter is to develop some notions of quantum mechanics, for which we devote the first two sections, to subsequently introduce and discuss the quantum mechanical analogues of what was previously seen.

The work by Kepler and later by Newton was crucial for the foundations of classical mechanics. However, as scientific exploration progressed, questions about particles in the microscopic realm arose. No longer was the classical theory sufficient enough to explain phenomena that were observed in that realm. That is were the theory of quantum mechanics came in to place. It is a theory that was not developed by one individual, but rather it is a collective work of many great physicists, the origin of which can be traced back to the early 20^{th} century. It rigorously explains behaviour of particles at the atomic scale. However, it must be said that such behaviour was often perceived as being peculiar and counter-intuitive, making it a challenge in itself to fully understand the framework.

An example of an object at the atomic scale, and hence ought to be examined quantum mechanically, is the hydrogen atom. It is the simplest atom in the periodic table consisting of just one proton and one electron. The latter are both electrically charged particles, and hence we find a force between them: the Coulomb force, see *Equation* (1.3). One can already see that this serves as a quantum analogue to the Sun-planet system. This will be considered more thoroughly in *Section* 2.3. Afterwards, we develop some quantum mechanical formalism needed for reviewing (hidden) symmetries.

2.1 Preliminaries from Quantum Mechanics

In this section, we present some important preliminaries from quantum mechanics. While doing so, we use the book by Griffiths [13] as a main source of inspiration. As such, this reference will only be explicitly stated when appropriate.

To bridge the gap between classical and quantum mechanics, recall that in *Chapter* 1 we considered classical point particles with a mass m. Suppose we have such a particle again moving in three-dimensional space. We can then determine the motion of the particle $\mathbf{r}(t) \in \mathbb{R}^3$, with $t \in \mathbb{R}$ denoting time, by using Newton's law $m\ddot{\mathbf{r}} = \mathbf{F}(\mathbf{r}, t)$ and some initial conditions. Although in quantum mechanics, we are still concerned with describing the particle, we

do so in terms of the wave function $\Psi(\mathbf{r}, t)$. This time, we use Schrodinger's equation, which we shall introduce in due time, also together with some initial conditions.

The possible states that a quantum mechanical system can be found in are referred to as quantum states. A quantum state is a vector, for that reason also called a state vector, and lives in a complex Hilbert space. For clarity and completeness, we include the definition of this space.

Definition 2.1.1 (Complex Hilbert space)**.** A **complex Hilbert space**[(ix)] $\mathcal{H}$ is a complex vector space with an inner product $\langle \cdot, \cdot \rangle$ such that the norm

$$\|f\| = \sqrt{\langle f, f \rangle}, \qquad f \in \mathcal{H}$$

turns $\mathcal{H}$ into a *complete metric space*[(x)].

Throughout the text, we make use of Dirac's 'braket' notation developed by Paul Dirac [26, 7]. In braket notation, we have *bra*'s and *ket*'s. A state vector is a ket, which is denoted as $|\Psi\rangle$, where Ψ is the wave function. On the other hand, $\langle\Psi|$ is called a bra, which we shall see more of shortly. In Dirac's notation, the inner product of two state vectors $|\psi\rangle, |\phi\rangle \in \mathcal{H}$, where $\mathcal{H}$ is a Hilbert space, is denoted by $\langle\psi|\phi\rangle \in \mathbb{C}$. The fact that the inner product is in general complex is because the vector space $\mathcal{H}$ is complex. Notice the notation of the inner product is essentially the merging of a bra and a ket, obtaining a braket. We say that a bra $\langle\psi|$ is an element of the dual of $\mathcal{H}$ which shall be denoted as $\mathcal{H}^*$. The correspondence between a ket $|\psi\rangle \in \mathcal{H}$ and its bra $\langle\psi| \in \mathcal{H}^*$ can easily be explicitly described by the Hermitian adjoint, see [20].

The state vector (or, ket) $|\Psi\rangle$ is fully specified by the wave function Ψ. We investigate some more what this wave function entails. Considering a particle moving in three dimensions, it is customary to take $\mathcal{H} = L^2(\mathbb{R}^3)$, i.e. the function space L^2 on $\mathbb{R}^3$ which consists of functions that are square-integrable in the whole of $\mathbb{R}^3$ [26]. We note that the inner product on $L^2(\mathbb{R}^3)$ is given by

$$\langle\psi|\phi\rangle = \int_{\mathbb{R}^3} \psi^*(\mathbf{r})\phi(\mathbf{r})\,\mathrm{d}^3\mathbf{r},$$

where $|\psi\rangle, |\phi\rangle \in L^2(\mathbb{R}^3)$. Here ψ^* denotes the conjugate of ψ. A common interpretation of wave function Ψ associated to the particle moving in three-dimensional space, where $|\Psi\rangle \in L^2(\mathbb{R}^3)$, is that

$$\int_\Delta |\Psi(\mathbf{r}, t)|^2\,\mathrm{d}^3\mathbf{r}$$

describes the probability of finding the particle in the region $\Delta \subseteq \mathbb{R}^3$ at time t. Here, $|\cdot|$ denotes the modulus, that is, $|\Psi(x,t)|^2 = \Psi^*(x,t)\Psi(x,t)$. We require

(ix) After this definition, we shall drop the specification that the Hilbert space is complex, and instead assume it always is complex.

(x) A metric space is said to be complete if every Cauchy sequence is convergent.

that the particle is somewhere and therefore

$$\langle \Psi | \Psi \rangle = \int_{\mathbb{R}^3} |\Psi(\mathbf{r}, t)|^2 \, \mathrm{d}\mathbf{r} = 1.$$

The process where one adjusts Ψ such that it adheres the above requirement is called *normalising*. An important realisation now is that whereas in a classical system Newton's laws together with suitable initial conditions allow us to comfortably describe the motion of a particle, the quantum mechanical approach is probabilistic in nature.

To each measurable parameter in a physical system, or, what is also called an observable, we associate a corresponding quantum mechanical operator. Examples of observables include the position and momentum of a particle. In a classical setting, we are used to $\mathbf{p} = m\mathbf{v}$, but the corresponding operator is obtained by the canonical substitution

$$p_{x_j} \to \frac{\hbar}{i} \frac{\partial}{\partial x_j}, \tag{2.1}$$

where $\hbar = h/(2\pi)$ with h being Planck's constant [13]. We now consider a more formal treatment of operators.

Definition 2.1.2 (Operators on $\mathcal{V}$)**.** Let $\mathcal{V}$ be a vector space. An **operator** on $\mathcal{V}$ is a map $\hat{A} : \mathcal{V} \to \mathcal{V}$ such that

$$\hat{A}(\lambda \left|\psi\right\rangle + \mu \left|\phi\right\rangle) = \lambda \hat{A}(\left|\psi\right\rangle) + \mu \hat{A}(\left|\phi\right\rangle),$$

for all $\lambda, \mu \in \mathbb{K}$ and $\left|\psi\right\rangle, \left|\phi\right\rangle \in \mathcal{V}$ (that is, the map is linear), where $\mathbb{K}$ is any field.

Consider the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)$, which in particular is a vector space. Then, the linear momentum operator on $\mathcal{H}$ is given by

$$\hat{\mathbf{P}} = \frac{\hbar}{i} \nabla.$$

Recall from *Chapter* 1 the Hamiltonian H, representing the total energy of a system. In quantum mechanics, the Hamiltonian is still of great importance. However, it is clear that now we do not talk about a function $H : (\mathbf{r}, \mathbf{p}) \mapsto p^2/(2m) + V(x)$ (classical Hamiltonian) but instead need to introduce the Hamiltonian as an operator on the Hilbert space $\mathcal{H}$. Using the operator $\hat{\mathbf{P}}$ on $\mathcal{H}$ as above, this can be quickly obtained:

$$\hat{H} = -\frac{\hbar^2}{2m} \underbrace{\sum_{j=1}^{3} \frac{\partial^2}{\partial x_j^2}}_{=:\nabla^2} + V(\mathbf{r}). \tag{2.2}$$

Here, ∇^2 denotes the Laplacian operator, also called the Laplacian for brevity, given in Cartesian coordinates. The above generalizes for $\mathcal{H} = L^2(\mathbb{R}^n)$, which is quickly established by looking at the canonical substitution in *Equation*

(2.1). In that case, the sum in $\hat{H}$ runs until n. (Also, notice that the potential energy V is assumed to be independent of t, as we shall assume throughout the text.)

Up until now, we considered the state vector $|\Psi(t)\rangle \in \mathcal{H}$ for a Hilbert space $\mathcal{H}$ to be specified by $\Psi(\mathbf{r}, t)$ with $\mathbf{r} \in \mathbb{R}^3$. But notice that implicitly a representation is chosen when mentioning the wave function $\Psi(\mathbf{r}, t)$ as such. More specifically, the position representation. But one could also use the momentum representation, see the definition below.

Definition 2.1.3 (Position and momentum representation)**.** Let $\mathcal{H}$ be a Hilbert space, then $\{|\mathbf{r}\rangle\}$ and $\{|\mathbf{p}\rangle\}$ are bases[(xi)] of $\mathcal{H}$ [9] which constitute the **position** and **momentum representation**, respectively. We define $\langle \mathbf{r} \,|\, \mathbf{r}' \rangle := \delta(\mathbf{r} - \mathbf{r}')$ and $\langle \mathbf{p} \,|\, \mathbf{p}' \rangle := \delta(\mathbf{p} - \mathbf{p}')$, where δ is the Dirac delta generalized function [29].

Using the definition, we can state the so-called *fundamental relations* [9]:

$$\langle \mathbf{r} \,|\, \mathbf{r}' \rangle = \delta(\mathbf{r} - \mathbf{r}') \qquad \langle \mathbf{p} \,|\, \mathbf{p}' \rangle = \delta(\mathbf{p} - \mathbf{p}'),$$
$$\int \mathrm{d}^3 r \, |\mathbf{r}\rangle \, \langle \mathbf{r}| = 1 \qquad \int \mathrm{d}^3 p \, |\mathbf{p}\rangle \, \langle \mathbf{p}| = 1.$$

Now for a given ket $|\Psi(t)\rangle \in \mathcal{H}$, it is possible to describe it in two forms, namely using the position representation and the momentum representation:

$$|\Psi\rangle = \int \mathrm{d}^3 r \, |\mathbf{r}\rangle \, \langle \mathbf{r} \,|\, \Psi \rangle \qquad \text{and} \qquad |\Psi\rangle = \int \mathrm{d}^3 p \, |\mathbf{p}\rangle \, \langle \mathbf{p} \,|\, \Psi \rangle \,,$$

where $\langle \mathbf{r} \,|\, \Psi \rangle = \Psi(\mathbf{r}, t)$ and $\langle \mathbf{p} \,|\, \Psi \rangle = \Psi^*(\mathbf{p}, t)$, see [9].

Returning to the concept of the wave function describing a particle, what is of course of interest is its time evolution. Consider the wave function Ψ where $|\Psi\rangle \in L^2(\mathbb{R}^3) =: \mathcal{H}$[(xii)]. The time evolution is determined by *Schrödinger's equation*:

$$i\hbar \frac{\partial}{\partial t} |\Psi(t)\rangle = \hat{H} \, |\Psi(t)\rangle \,,$$

with the Hamiltonian operator $\hat{H}$ as in *Equation* (2.2). To see how to solve the Schrödinger equation in three dimensions, it is instructive to first look at how it can be solved in one dimension. In the latter case, Schrödinger's equation fully written out in the position representation looks like:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \frac{\partial^2 \Psi}{\partial x^2} + V\Psi.$$

Using separation of variables, the wave function can be written as $\Psi(x, t) = \psi(x)\varphi(t)$ where ψ is a function solely of x and φ solely of t. Then, the above

[(xi)] The generalised function δ does not belong to $\mathcal{H}$, but we can safely ignore this. See [9].

[(xii)] Dimension three is picked since this was used exclusively in the previous chapter, and will be considered below, but in fact any dimension n can be chosen here.

becomes

$$\begin{aligned} i\hbar\psi\frac{\mathrm{d}\varphi}{\mathrm{d}t} &= -\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2}\varphi + V\psi\varphi \\ \Rightarrow i\hbar\frac{1}{\varphi}\frac{\mathrm{d}\varphi}{\mathrm{d}t} &= -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V. \end{aligned}$$

While the left hand side depends only on t, we find that the right hand side only depends on x. But this means that both sides must in fact be constant (so in particular independent of x and t). The separation constant we call E, so

$$i\hbar\frac{1}{\varphi}\frac{\mathrm{d}\varphi}{\mathrm{d}t} = E \qquad \text{and} \qquad -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V = E. \tag{2.3}$$

The first can be quickly solved, namely

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = -\frac{i}{\hbar}E\varphi \qquad \Rightarrow \qquad \varphi(t) = \exp\left(-\frac{i}{\hbar}Et\right).$$

The second equation of *Equation* (2.3) can be rewritten by multiplying both sides with ψ:

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2\psi}{\mathrm{d}x^2} + V\psi = E\psi. \tag{2.4}$$

We call this the time-independent Schrödinger equation. In order to solve it, the potential V needs to be specified. So instead let's take a step back and examine the separable solutions. To this end, consider the wave function $\Psi(x,t) = \psi(x)\exp(-iEt/\hbar)$ which depends on t. We have that

$$\begin{aligned} |\Psi(x,t)|^2 &= \Psi^*(x,t)\Psi(x,t) \\ &= \psi(x)^*\exp(+iEt/\hbar)\psi(x)\exp(-iEt/\hbar) \\ &= |\psi(x)|^2. \end{aligned}$$

That is, $|\Psi(x,t)|^2$ turns out to be independent of time. We will keep this result in mind, and come back to it when it is needed directly after the following definition.

Definition 2.1.4 (Expectation value)**.** In the position representation, an observable $\mathcal{Q}(x,p)$ has **expectation value**

$$\langle\mathcal{Q}(x,p)\rangle := \langle\Psi \mid \hat{\mathcal{Q}}\Psi\rangle = \int \Psi^*\hat{\mathcal{Q}}\left(x, \frac{\hbar}{i}\frac{\partial}{\partial x}\right)\Psi\,\mathrm{d}x, \tag{2.5}$$

where $\hat{\mathcal{Q}}$ is the operator on $\mathcal{H} := L^2(\mathbb{R})$ corresponding to the observable $\mathcal{Q}$[(xiii)].

The behaviour of $|\Psi(x,t)|^2$ being independent of t is also seen in the expectation value of any $\mathcal{Q}(x,p)$ [13]. That means *Equation* (2.5) can be rewritten

[(xiii)] To every observable $\mathcal{Q}$, there is a corresponding *Hermitian* operator $\hat{\mathcal{Q}}$. This will be explained more carefully in *Section* 2.4.

using just ψ:

$$\langle \mathcal{Q}(x,p) \rangle = \int \psi^* \hat{\mathcal{Q}} \left(x, \frac{\hbar}{i} \frac{\partial}{\partial x} \right) \psi \, \mathrm{d}x.$$

In order to obtain the expectation value of the total energy, $\langle H \rangle$, we rewrite *Equation* (2.4) using the Hamiltonian operator $\hat{H}$:

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

We then find that

$$\langle H \rangle = \int \psi^* \hat{H} \psi \, \mathrm{d}x = \int E \underbrace{\psi^* \psi}_{=|\psi|^2} \, \mathrm{d}x = E \int |\Psi|^2 \, \mathrm{d}x = E,$$

by using $|\Psi(x,t)|^2 = |\psi(x)|^2$ and the fact that Ψ is normalised (also, normalisation of Ψ encompasses normalisation of ψ). See [13, *Section* 2.1] where it is shown that for separable solutions, every measurement of the total energy is certain to return E by calculating the variance. It now makes sense why the notation E for the separation constant was chosen. A last important property of the separable solutions is that the general solution of the wave function is a linear combination of these separable solutions. The time-independent Schrödinger equation $\hat{H}\psi = E\psi$ has solutions $\psi_1(x), \psi_2(x), \psi_3(x), \ldots$ and to each of them there is an associated separation constant E_i, $i \in \mathbb{Z}_{>0}$. This yields *stationary states*

$$\Psi_1(x,t) = \psi_1(x) \exp\left(-\frac{i}{\hbar} E_1 t \right), \qquad \Psi_2(x,t) = \psi_2(x) \exp\left(-\frac{i}{\hbar} E_2 t \right), \qquad \ldots .$$

So we have a different wave function for each E_i, which we call the allowed energies. Since any linear combination of solutions to the Schrödinger equation is a solution, we conclude that

$$\begin{aligned} \Psi(x,t) &= \sum_{n=1}^{\infty} c_n \Psi_n(x,t) \\ &= \sum_{n=1}^{\infty} c_n \psi_n(x) \exp\left(-\frac{i}{\hbar} E_i t \right), \end{aligned}$$

where c_n are coefficients, and $i \in \mathbb{Z}_{>0}$. These coefficients are determined by the initial wave function $\Psi(x,0)$.

2.2 The Schrödinger Equation in 3D

We now consider the Schrödinger equation in three dimensions, where we shall make use of spherical coordinates. Consider the Hilbert space $\mathcal{H} = L^2(\mathbb{R}^3)$, and recall that the momentum operator is $\hat{\mathbf{P}} = (\hbar/i)\nabla$. The Schrödinger equation is then given by

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V\Psi,$$

where $|\Psi\rangle \in \mathcal{H}$. Let $\mathbf{r} = (x, y, z)$ be the position. The normalisation requirement seen before, which we shall now write in a slightly di□erent manner, is

$$\iiint_{\mathbb{R}^3} |\Psi(\mathbf{r}, t)|^2 \, \mathrm{d}x\mathrm{d}y\mathrm{d}z = 1. \tag{2.6}$$

Moreover, the stationary states are given by

$$\Psi_n(\mathbf{r}, t) = \psi_n(\mathbf{r}) \exp\left(-\frac{i}{\hbar} E_n t\right),$$

where $n \in \mathbb{Z}_{>0}$ and ψ_n satisfy $\hat{H}\psi = E\psi$ with $\hat{H}$ the Hamiltonian operator for three dimensions as seen in *Equation* (2.2). Having the stationary states, we find that, completely analogously to the one-dimensional case, the time-dependent Schrödinger equation has general solution

$$\Psi(\mathbf{r}, t) = \sum_{n=1}^{\infty} c_n \psi_n(\mathbf{r}) \exp\left(-\frac{i}{\hbar} E_n t\right),$$

with c_n coe□cients determined by $\Psi(\mathbf{r}, 0)$, and $i \in \mathbb{Z}_{>0}$.

Since it is usual for the potential V to only depend on the distance from the origin, it is intuitive to use spherical coordinates (ρ, θ, ϕ) where ρ is the radius, θ is the polar angle, and ϕ is the azimuthal angle. Then $V(\rho)$ is the potential. In spherical coordinates, the Laplacian becomes [13]

$$\nabla^2 = \frac{1}{\rho^2}\frac{\partial}{\partial \rho}\left(\rho^2 \frac{\partial}{\partial \rho}\right) + \frac{1}{\rho^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial}{\partial \theta}\right) + \frac{1}{\rho^2 \sin^2\theta}\left(\frac{\partial^2}{\partial \phi^2}\right). \tag{2.7}$$

Substituting this in the time-independent Schrödinger equation $\hat{H}\psi = E\psi$ where $\hat{H} = -(\hbar^2/(2m))\nabla^2 + V(\rho)$ gives

$$-\frac{\hbar^2}{2m}\left[\frac{1}{\rho^2}\frac{\partial}{\partial \rho}\left(\rho^2 \frac{\partial \psi}{\partial r}\right) + \frac{1}{\rho^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial \psi}{\partial \theta}\right) + \frac{1}{\rho^2 \sin^2\theta}\left(\frac{\partial^2 \psi}{\partial \phi^2}\right)\right] + V\psi = E\psi. \tag{2.8}$$

Employing the same separation by variables technique seen before, we let

$$\psi(\rho, \theta, \phi) = R(\rho)Y(\theta, \phi),$$

where R solely depends on the radius ρ, while Y solely depends on the angles θ and ϕ. Therefore *Equation* (2.8) becomes, by substituting,

$$-\frac{\hbar^2}{2m}\left[\frac{Y}{\rho^2}\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho^2 \frac{\mathrm{d}R}{\mathrm{d}\rho}\right) + \frac{R}{\rho^2 \sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta \frac{\partial Y}{\partial \theta}\right) + \frac{R}{\rho^2 \sin^2\theta}\left(\frac{\partial^2 Y}{\partial \phi^2}\right)\right] + VRY = ERY.$$

Subsequently, rewriting gives

$$\underbrace{\left[\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho^2\frac{\mathrm{d}R}{\mathrm{d}\rho}\right)-\frac{2m}{\hbar^2}\left(V(\rho)-E\right)\right]}_{\text{Depends only on } \rho} + \underbrace{\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right]}_{\text{Depends only on } \theta \text{ and } \phi} = 0.$$

Similar to the one-dimensional case, since the first term only depends on ρ and the second on θ and ϕ, it is concluded that both terms must be constant. We introduce the separation constant $l(l+1)$, where $l \in \mathbb{C}$. This might look peculiar at first, but nonetheless turns out to be correct. So for convenience we already adopt this form. We refer to [13, 9] for more details. Note that we do not restrict l. We now have

$$\left[\frac{1}{R}\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho^2\frac{\mathrm{d}R}{\mathrm{d}\rho}\right)-\frac{2m}{\hbar^2}\left(V(\rho)-E\right)\right] = l(l+1), \tag{2.9}$$

and

$$\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] = -l(l+1). \tag{2.10}$$

At this point, we rely on separation of variables once more, now for the angular function Y. Let $Y(\theta,\phi) = \Theta(\theta)\Phi(\phi)$, then *Equation* (2.10) becomes:

$$\underbrace{\left[\frac{1}{\Theta}\left(\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)\right)+l(l+1)\sin^2\theta\right]}_{\text{Depends only on } \theta} + \underbrace{\frac{1}{\Phi}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2}}_{\text{Depends only on } \phi} = 0.$$

So, both terms must be constant. Let the separation constant be of the form m^2, where initially $m \in \mathbb{C}$[(xiv)]. Again, see [13] for relevant details. Then:

$$\frac{1}{\Theta}\left(\sin\theta\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)\right)+l(l+1)\sin^2\theta = m^2, \tag{2.11}$$

and

$$\frac{1}{\Phi}\frac{\mathrm{d}^2\Phi}{\mathrm{d}\phi^2} = -m^2.$$

The latter is readily solved, namely $\Phi(\phi) = \exp(im\phi)$. Notice that Φ must be 2π-periodic since $\phi \in [0, 2\pi)$ is the azimuthal angle. That is, $\Phi(\phi+2\pi) = \Phi(\phi)$, so it follows that $\exp(im(\phi+2\pi)) = \exp(im\phi)$ and hence $\Phi(2\pi im) = 1$. It then becomes clear that we must have $m \in \mathbb{Z}$, i.e., m is an integer.

[(xiv)] This m, coming from the separation constant, should not be confused with mass.

On the other hand, solving *Equation* (2.11), requires some more effort. First, notice that the equation can be rewritten as

$$\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}\Theta}{\mathrm{d}\theta}\right)-\frac{m^2}{\sin^2\theta}\Theta+l(l+1)\Theta=0. \tag{2.12}$$

In order to find the solution, consider the following definition.

Definition 2.2.1 (Associated Legendre polynomials)**.** Let $l\in\mathbb{Z}_{\geq 0}$. The *Legendre polynomials*, denoted by $P_l(\cos\theta)$, are given by

$$P_l(\cos\theta)=\frac{1}{2^l l!}\frac{\mathrm{d}^l}{(\mathrm{d}\cos\theta)^l}(\cos^2\theta-1)^l,$$

and they satisfy the differential equation

$$\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}P_l}{\mathrm{d}\theta}\right)l(l+1)P_l=0.$$

Then, the **associated Legendre functions**[(xv)], denoted by $P_l^m(\cos\theta)$, are defined by

$$P_l^m(\cos\theta)=\sin^m\theta\frac{\mathrm{d}^m P_l(\cos\theta)}{(\mathrm{d}\cos\theta)^m},$$

where $m\in\{0,1,\ldots,l\}$. The functions $P_l^m(\cos\theta)$ satisfy the differential equation

$$\frac{1}{\sin\theta}\frac{\mathrm{d}}{\mathrm{d}\theta}\left(\sin\theta\frac{\mathrm{d}P_l^m}{\mathrm{d}\theta}\right)-\frac{m^2}{\sin^2\theta}P_l^m+l(l+1)P_l^m=0.$$

With m and l as in the definition, we have that P_l^m and P_l^{-m} are related by[(xvi)] [30]

$$P_l^{-m}(\cos\theta)=(-1)^m\frac{(l-m)!}{(l+m)!}P_l^m(\cos\theta).$$

For more details on (associated) Legendre functions, we refer to *Chapter* IV and *Appendix* §c of [25]. Equipped with these functions, it becomes apparent that *Equation* (2.12) has solution

$$\Theta(\theta)=CP_l^m(\cos\theta),$$

[(xv)] In literature, (for example [25]) these are often called associated Legendre *polynomials*. However, while m is odd, P_l^m is not a polynomial. Furthermore, to avoid confusion, note that we do not refer to the so-called associated Legendre functions of the second kind.

[(xvi)] There is a sign convention for defining the associated Legendre functions. We chose to omit the phase factor $(-1)^m$, so one might ask why it is present here. This is best seen by considering the associated Legendre functions in the form

$$P_l^m(x)=\frac{1}{2^l l!}(1-x^2)^{\frac{m}{2}}\frac{\mathrm{d}^{l+m}}{\mathrm{d}x^{l+m}}(x^2-1)^l,$$

and then applying Leibniz's differentiation rule. Also see [22].

where C is constant, and P_l^m are the associated Legendre functions with $|m| \leq l$, $m \in \mathbb{Z}$, and $l \in \mathbb{Z}_{\geq 0}$. Notice that for a given l there are $(2l+1)$ possible values m can take.

We now have solutions for Θ and Φ, which were the separated functions of Y. Notice that Θ depends on m and l, so we write Θ_l^m for Θ and Y_l^m for Y. That is:

$$Y_l^m = \Theta_l^m(\theta)\Phi(\phi).$$

We can work towards giving solutions of Y_l^m, but we want to give *normalised* solutions, so to that end consider the normalisation requirement given in *Equation* (2.6). By change of variables for integrals, it is translated to

$$\begin{aligned} 1 &= \int_0^{2\pi}\int_0^{\pi}\int_0^{\infty} |\psi(\rho,\theta,\phi)|^2 \rho^2 \sin\theta \,\mathrm{d}\rho\mathrm{d}\theta\mathrm{d}\phi \\ &= \int_0^{\infty} |R(\rho)|^2 \rho^2 \,\mathrm{d}\rho \int_0^{2\pi}\int_0^{\pi} |Y_l^m(\theta,\phi)|^2 \sin\theta \,\mathrm{d}\theta\mathrm{d}\phi \end{aligned}$$

when using spherical coordinates since $\mathrm{d}x\mathrm{d}y\mathrm{d}z = \rho^2 \sin\theta \mathrm{d}\rho\mathrm{d}\theta\mathrm{d}\phi$. The radial function R and angular function Y can be normalised separately, so one obtains for normalising Y_l^m the following:

$$\int_0^{2\pi}\int_0^{\pi} |Y_l^m(\theta,\phi)|^2 \sin\theta \,\mathrm{d}\theta\mathrm{d}\phi = 1.$$

Now the normalised solutions of $Y_l^m = \Theta_l^m\Phi$ can be given, see below.

Definition 2.2.2 (Spherical harmonics)**.** The solutions of $Y_l^m(\theta,\phi)$ are called **spherical harmonics** and are given by [22]

$$Y_l^m(\theta,\phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}} \exp(im\phi) P_l^m(\cos\theta), \tag{2.13}$$

where $(-1)^m$ is called the Condon-Shortley phase factor, and P_l^m are the associated Legendre functions. Here, $m \in \mathbb{Z}$ such that $|m| \leq l$ is the magnetic quantum number, and $l \in \mathbb{Z}_{\geq 0}$ is the azimuthal quantum number.

In *Figure* 2.1 below, a sample of these spherical harmonics Y_l^m are drawn.

Considering the spatial part of the wave function, $\psi(\rho,\theta,\phi) = R(\rho)Y_l^m(\theta,\phi)$, it can be seen that the potential $V(\rho)$, which is assumed to be independent of t, only has an e□ect on the radial function $R(\rho)$ which is obtained by *Equation* (2.9), which after multiplying by R looks like

$$\frac{\mathrm{d}}{\mathrm{d}\rho}\left(\rho^2 \frac{\mathrm{d}R}{\mathrm{d}\rho}\right) - \frac{2m}{\hbar^2}\left(V(\rho) - E\right) R = l(l+1)R.$$

If we let $u(\rho) = \rho R(\rho)$, then the above becomes

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2 u}{\mathrm{d}\rho^2} + \left(V(\rho) + \frac{\hbar^2}{2m}\frac{l(l+1)}{\rho^2}\right) u = Eu. \tag{2.14}$$

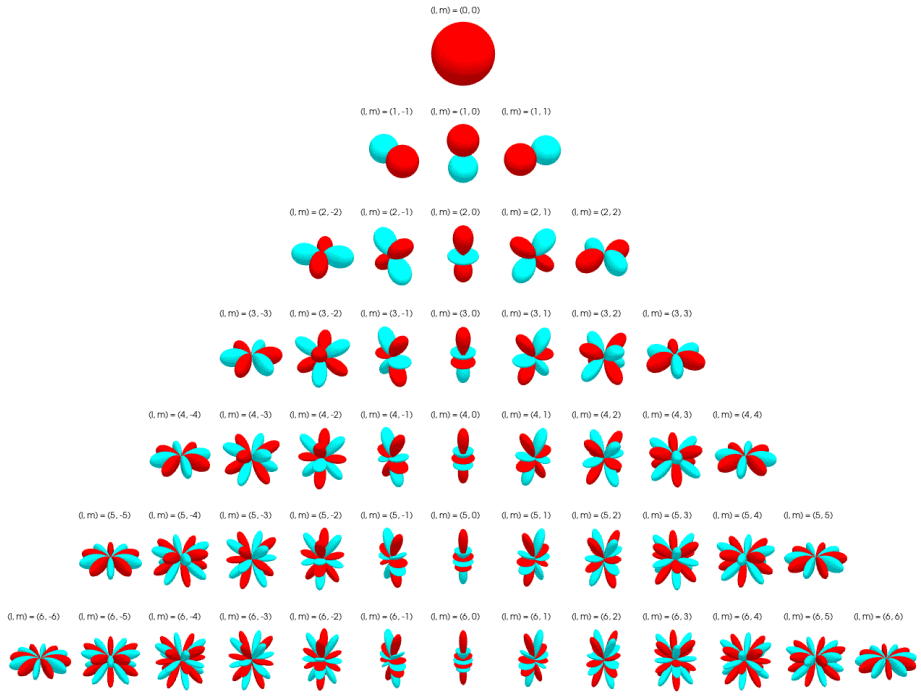

Figure 2.1: Polar plots of the spherical harmonics Y_l^m for $m \in \{-6, \ldots, -1, 0, 1, \ldots, 6\}$ and $l \in \{0, 1, 2 \ldots, 6\}$. The magnitude of each Y_l^m corresponds to the radius. Taken from [10].

This equation seems familiar, and indeed it has the form of the time-independent Schrödinger equation given in *Equation* (2.4). What di□ers is the extra

$$\frac{\hbar^2}{2m}\left(\frac{l(l+1)}{\rho^2}\right)$$

part in *Equation* (2.14), which we call the *centrifugal term*. We define the *e ective potential* to be the sum of the potential $V(\rho)$ and this centrifugal term, that is,

$$V_{\text{e}\square}(\rho) := V(\rho) + \frac{\hbar^2}{2m}\frac{l(l+1)}{\rho^2}. \tag{2.15}$$

2.3 Hydrogen Atom

Any atom can be described as a nucleus with positive charge $+Ze$, and Z electrons orbiting the nucleus where each electron has a charge of $-e$. We consider the simplest atom, being the hydrogen atom in which case $Z = 1$. The force between the nucleus and the electron is described by Coulomb's force, which was already introduced in *Chapter* 1, see *Equation* (1.3), as part of a particular instance of the Kepler problem. In the hydrogen atom, the nucleus, consisting of a single proton, has charge $+e$ and the electron $-e$, also see *Figure* 2.2. If we say that the vector $\mathbf{r}$ connects the proton with the electron, we have

that Coulomb's force is given by

$$\mathbf{F} = -\frac{1}{4\pi\varepsilon_0}\frac{e^2}{r^3}\,\mathbf{r},$$

where the constant ε_0 is the permittivity of free space.

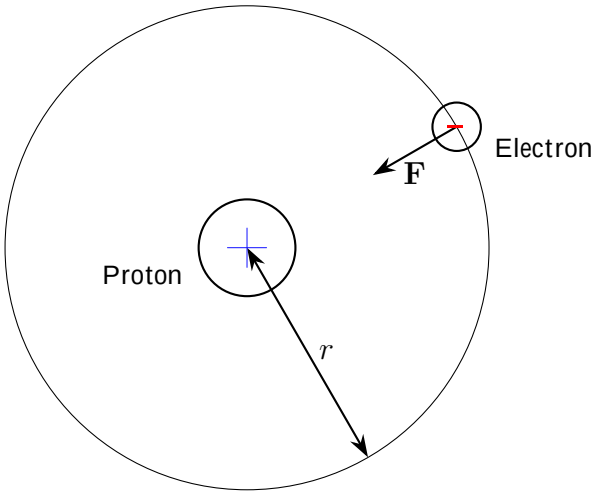

Figure 2.2: Schematic view of the hydrogen atom, here $\mathbf{F}$ is the Coulomb force.

From this force, we can obtain the potential energy V since $\mathbf{F} = -\nabla V$. So it can be seen that

$$V(\mathbf{r}) = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}. \tag{2.16}$$

We call this the *Kepler potential*. We have now established what the quantum Kepler problem in three dimensions looks like. By using the Kepler potential, it follows that the e□ective potential as defined in *Equation* (2.15), in spherical coordinates, is

$$V_{\text{e}\square}(\rho) = -\frac{e^2}{4\pi\varepsilon_0}\frac{1}{\rho} + \frac{\hbar^2}{2m}\frac{l(l+1)}{\rho^2}.$$

Using *Equation* (2.14) we can obtain the allowed energies E_n, where $n \in \mathbb{Z}_{>0}$. That is, one needs to solve

$$-\frac{\hbar^2}{2m}\frac{\mathrm{d}^2u}{\mathrm{d}\rho^2} + \left(-\frac{e^2}{4\pi\varepsilon_0}\frac{1}{\rho} + \frac{\hbar^2}{2m}\frac{l(l+1)}{\rho^2}\right)u = Eu$$

for $u(\rho)$, and find the allowed energies. For a full derivation, we refer to [13, *Section* 4.2]. The allowed energies, which we shall look at more closely now, turns out to be given by

$$\begin{aligned} E_n &= -\left[\frac{m_e}{2\hbar^2}\left(\frac{e^2}{4\pi\varepsilon_0}\right)^2\right]\frac{1}{n^2} \\ &= -\frac{m_e e^4}{32\pi^2\varepsilon_0^2\hbar^2}\frac{1}{n^2}, \end{aligned}$$

also referred to as Bohr's formula[(xvii)]. The lowest energy possible is the ground state where $E_1 = -13.6$ eV (electronvolt)[(xviii)]. The (electron) binding energy of an atom is the energy required to separate the atom into free electrons and nucleus (shortly described as ionising). The binding energy of the hydrogen atom is 13.6 eV. Notice that E_n can also be written as $E_n = E_1/n^2$. So, $E_2 = -13.6/4 = -3.4$ eV. This means it takes less energy to ionise the hydrogen atom when it is in the second energy level. To emphasise its importance, note that the electron of a hydrogen atom *cannot* have energies between E_1 and E_2, it is said to be *quantised*. All energies E_n with $n \in \mathbb{Z}_{>0}$ that can be obtained with Bohr's formula are negative and are belonging to so-called bound states. However, the Schrödinger equation also has solutions with positive energies. These solutions correspond to the physical states where the electron is free of the nucleus after being ejected by a high-energy collision or a photon, also called unbound states. We shall not concern ourselves with those any further.

Recall the spatial wave function $\psi = RY_l^m(\theta, \phi)$. Because of the quantised nature of the energy levels E_n, $n \in \mathbb{Z}_{>0}$, we call n the principal quantum number. To that end, we write $R_{n,l}$ for R due to its dependence on both n and l. (Y is independent of n, so we leave it as Y_l^m.) From *Equation* (2.14) we gathered the allowed energies E_n, but moreover $R_{n,l}$ can be obtained, since $u(r) = rR_{n,l}(r)$. This results in

$$R_{n,l}(\rho) = \frac{1}{\rho}\omega^{l+1}\exp(-\omega)v(\omega), \qquad \omega = \frac{\rho}{n}\frac{1}{a_0}, \qquad a_0 = \frac{4\pi\varepsilon_0\hbar^2}{m_e e^2}. \tag{2.17}$$

Here, $v(\omega)$ is a polynomial of degree $n-l-1$ with coefficients (up to normalisation)

$$c_{j+1} = \frac{2(j+l+1-n)}{(j+1)(j+2l+2)}c_j, \qquad j \in \{0, 1, \ldots, n-l-1\}.$$

The coefficient c_0 is determined by normalising. We say a_0 in *Equation* (2.17) is the Bohr radius which describes the maximum probable distance between the nucleus and the electron in the ground state of a hydrogen atom [32]. We now find ourselves in a position where we can fully solve the spatial wave function:

$$\psi_{n,l,m}(\rho, \theta, \phi) = R_{n,l}(\rho)Y_l^m(\theta, \phi).$$

Here, $R_{n,l}$ is given by *Equation* (2.17) and Y_l^m (the spherical harmonics) by *Equation* (2.13). So we can for example explicitly describe the ground state

(xvii) In *Chapter* 1, we introduced the reduced mass μ when dealing with celestial bodies. One could do the same here, but since the mass of the electron is negligible compared to that of the proton, $m_p \gg m_e$, we find that the reduced mass is almost the same as the mass of the electron:

$$\mu = \frac{m_p m_e}{m_p + m_e} \approx 0.9995 m_e.$$

We note that when doing laboratory experiments this difference, although minor, should be taken into account. For our purposes we ignore this, and instead choose to only write the mass of the electron, something that is often seen in literature.

(xviii) See https://physics.nist.gov/cuu/Constants for values of m_e (electron mass), e (elementary charge), $\hbar$ (reduced Planck constant), and ε_0 (permittivity of free space).

of the hydrogen atom, which is $\psi_{1,0,0} = R_{1,0}Y_0^0$. The radial function is given by $R_{1,0}(\rho) = (c_0/a_0)\exp(-\rho/a_0)$, which after normalising becomes $R_{1,0}(\rho) = (2/a_0^{3/2})\exp(-\rho/a_0)$. The spherical harmonic function is $Y_0^0 = 1/\sqrt{4\pi}$, so $\psi_{1,0,0}$ yields

$$\psi_{1,0,0}(\rho,\theta,\phi) = \frac{1}{\sqrt{\pi a_0^3}}\exp\left(-\frac{\rho}{a_0}\right).$$

An electron in the ground state can be visualised in *Figures* 2.3 and 2.4 below.

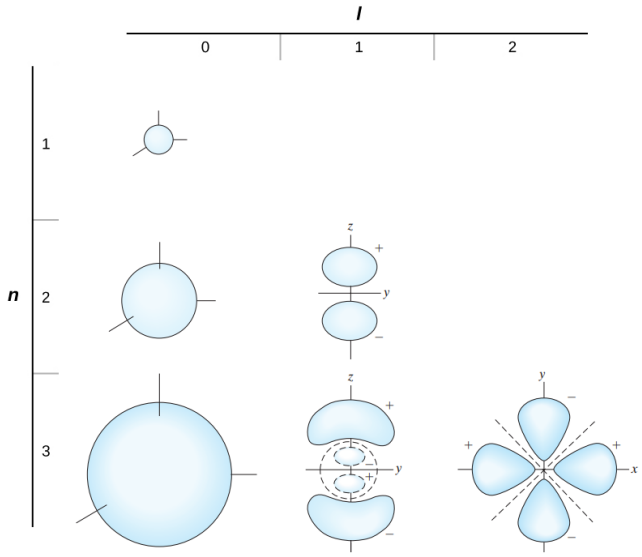

Figure 2.3: Shapes of the orbitals for various states of the hydrogen atom. Taken and amended from [28].

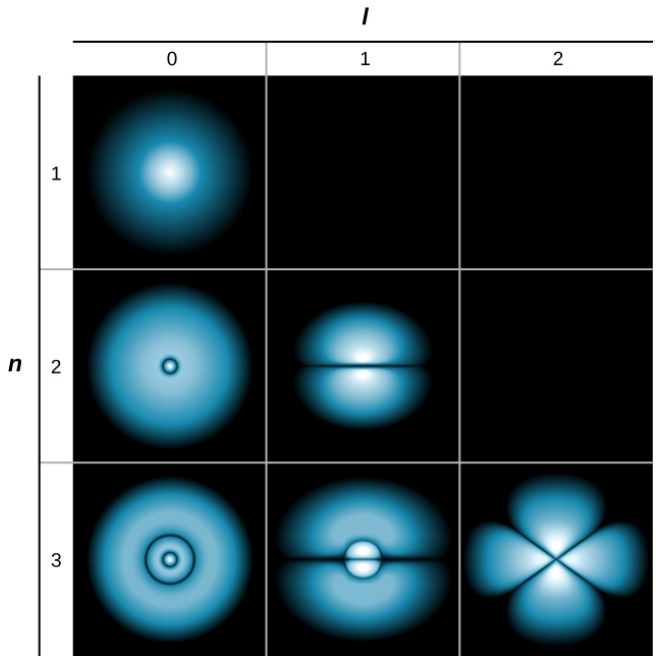

Figure 2.4: Probability densities for various states of the hydrogen atom. Taken from [36].

2.4 Complete Sets of Commuting Observables

Throughout this section, we consider $\mathcal{H}$ to be a Hilbert space satisfying the following additional conditions [26]:

I. Only $|\psi\rangle \in \mathcal{H}$ with $\langle\psi|\psi\rangle = 1$ correspond to physical states,

II. Kets di□ering by a phase, i.e. $|\psi\rangle$ and $\exp(i\theta)\,|\psi\rangle$ where $\theta \in \mathbb{R}$, correspond to the *same* physical states.

What this means, is that in quantum mechanics the state space is not just a Hilbert space $\mathcal{H}$ but in fact the projective Hilbert space $\mathcal{P}(\mathcal{H})$ which is defined as $S\mathcal{H}/\sim$ where

$$S\mathcal{H} := \{|\psi\rangle \in \mathcal{H} \mid \langle\psi|\psi\rangle = 1\} \qquad \text{and} \qquad |\psi\rangle \sim |\phi\rangle \iff |\psi\rangle = z\,|\phi\rangle\,,\ z \in \mathbb{C}.$$

For our purposes, we do not write $\mathcal{P}(\mathcal{H})$, but, equivalently, it is understood that a Hilbert space $\mathcal{H}$ satisfies (I) and (II). Moreover, while generally $\mathcal{H}$ is left unspecified, we assume that $\mathcal{H} = L^2(\mathbb{R}^n)$ unless mentioned otherwise (the dimension n usually follows from the context). Lastly, another remark is that we implicitly assume that for an eigenket $|\psi\rangle$ we have $|\psi\rangle \in \mathcal{H}$, and that an operator $\hat{A}$ is always on $\mathcal{H}$.

The Hamiltonian for the hydrogen atom system is obtained by combining the general expression for $\hat{H}$ given in *Equation* (2.2) with the Kepler potential described in *Equation* (2.16):

$$\hat{H} = -\frac{\hbar^2}{2m_e}\nabla^2 - \frac{e^2}{4\pi\varepsilon_0}\frac{1}{r}, \tag{2.18}$$

where by m_e we denote the mass of the electron[(xix)].

We now provide a very crucial definition, the concept of which turns out to be fundamental in quantum mechanics.

Definition 2.4.1 (Commutator)**.** Let $\hat{A}, \hat{B}$ be operators. Then the **commutator** of these operators is

$$\left[\hat{A}, \hat{B}\right] := \hat{A}\hat{B} - \hat{B}\hat{A}.$$

We say that $\hat{A}$ and $\hat{B}$ *commute* if $\left[\hat{A}, \hat{B}\right] = 0$.

As an example, let $|\psi\rangle$ be arbitrary with corresponding wave function in the $\{|\mathbf{r}\rangle\}$ representation $\psi(\mathbf{r}) = \langle\mathbf{r}\,|\,\psi\rangle$, where $\mathbf{r} = (x, y, z) \in \mathbb{R}^3$. Consider the operator $\hat{R}_x : |\psi\rangle \mapsto |\psi'\rangle$ which is represented in $\{|\mathbf{r}\rangle\}$ by $\psi'(\mathbf{r}) = \langle\mathbf{r}\,|\,\psi'\rangle$ such that $\psi'(\mathbf{r}) = x\psi(\mathbf{r})$ [9]. Therefore, we have

$$\hat{R}_x : \psi(\mathbf{r}) \mapsto \psi'(\mathbf{r}) := x\psi(\mathbf{r}). \tag{2.19}$$

[(xix)] For reasons discussed earlier, we do not consider the reduce mass here. In essence, this is because the the mass of the electron being negligible compared to that of the proton. If preferred, one can quite easily, mutatis mundatis, work with the reduced mass in the Hamiltonian for the hydrogen atom.

Analogously, operators $\hat{R}_y$ and $\hat{R}_z$ are given by $\hat{R}_y : \psi(\mathbf{r}) \mapsto y\psi(\mathbf{r})$ and $\hat{R}_z : \psi(\mathbf{r}) \mapsto z\psi(\mathbf{r})$, respectively. On the other hand, let the momentum operator of x_j in the $\{|\mathbf{r}\rangle\}$ representation be given by

$$\hat{P}_{x_j} : \psi(\mathbf{r}) \mapsto \frac{\hbar}{i}\frac{\partial}{\partial x_j}\psi(\mathbf{r}), \tag{2.20}$$

where $j \in \{1, 2, 3\}$, which is obtained from *Equation* (2.1). It then follows that, for an arbitrary $\psi(\mathbf{r})$,

$$\begin{aligned}
\left[\hat{R}_x, \hat{P}_x\right]\psi(\mathbf{r}) &= \left(\hat{R}_x\hat{P}_x - \hat{P}_x\hat{R}_x\right)\psi(\mathbf{r}) \\
&= \left(\hat{R}_x\hat{P}_x\right)\psi(\mathbf{r}) - \left(\hat{P}_x\hat{R}_x\right)\psi(\mathbf{r}) \\
&= \hat{R}_x\left(\hat{P}_x\psi(\mathbf{r})\right) - \hat{P}_x\left(\hat{R}_x\psi(\mathbf{r})\right) \\
&= x\frac{\hbar}{i}\frac{\partial}{\partial x}\left(\psi(\mathbf{r})\right) - \frac{\hbar}{i}\frac{\partial}{\partial x}\left(x\psi(\mathbf{r})\right) \\
&= \frac{\hbar}{i}\left(x\frac{\partial\psi(\mathbf{r})}{\partial x} - x\frac{\partial\psi(\mathbf{r})}{\partial x} - \psi(\mathbf{r})\right) \\
&= -\frac{\hbar}{i}\psi(\mathbf{r}) \\
&\boxed{= i\hbar\psi(\mathbf{r})}.
\end{aligned}$$

Since $\psi(\mathbf{r})$ was arbitrarily taken, we conclude that

$$\left[\hat{R}_x, \hat{P}_x\right] = i\hbar,$$

meaning $\hat{R}_x$ and $\hat{P}_x$ do not commutative. In a similar manner, we can obtain commutators [9]

$$\left[\hat{R}_i, \hat{R}_j\right] = 0, \qquad \left[\hat{P}_i, \hat{P}_j\right] = 0, \quad \text{and} \quad \left[\hat{R}_i, \hat{P}_j\right] = i\hbar\delta_i^j, \tag{2.21}$$

where $i, j \in \{1, 2, 3\}$, and $\hat{R}_1, \hat{R}_2, \hat{R}_3$ correspond to $\hat{R}_x, \hat{R}_y, \hat{R}_z$ respectively, and similarly $\hat{P}_1, \hat{P}_2, \hat{P}_3$ correspond to $\hat{P}_x, \hat{P}_y, \hat{P}_z$ respectively[(xx)]. Moreover, δ_i^j is Kronecker's delta for which $\delta_i^j = 1$ if $i = j$ and $\delta_i^j = 0$ if $i \neq j$. This result is called the *canonical commutation relations*, and is fundamental in quantum mechanics as a lot of its 'mysteries' can be traced to the non-commutativity of $\hat{R}_i$ with $\hat{P}_i$, which is why some authors choose to take this fact as an axiom [13].

By an abuse of notation, we often write commutation relation such as the first of *Equation* (2.21) as

$$\left[\hat{\mathbf{R}}, \hat{\mathbf{R}}\right] = 0, \tag{2.22}$$

where it is then understood that each pair $\hat{R}_i$, $\hat{R}_j$ commutes, $i, j \in \{1, 2, 3\}$.

[(xx)] This is a convention we shall adopt throughout the text without further mention.

Definition 2.4.2 (Hermitian adjoint and operator)**.** Let $\hat{A}$ be an operator. Its **Hermitian adjoint** is denoted by $\hat{A}^\dagger$ and is the unique operator such that

$$\langle \hat{A}\psi \,|\, \phi \rangle = \langle \phi \,|\, \hat{A}^\dagger \psi \rangle \,,$$

for all $|\psi\rangle, |\phi\rangle \in \mathcal{H}$ [4]. The operator $\hat{A}$ is said to be a **Hermitian operator** if $\hat{A}^\dagger = \hat{A}$.

An observable $\mathcal{Q}$ always has a corresponding Hermitian operator $\hat{\mathcal{Q}}$ [13]. So, in particular, $\hat{\mathbf{R}}$ and $\hat{\mathbf{P}}$ are Hermitian.

We now move over to the notion of angular momentum in quantum mechanics. In *Chapter* 1 it was seen that angular momentum, denoted by $\mathbf{L}$, played a crucial role when working in a classical setting. More specifically, it was shown that $\mathbf{L}$ is conserved in the isolated two-body problem, and that this implies Kepler's second law. Our attention will now lay on the quantum mechanical equivalents of those properties. First of all, to the classical angular momentum $\mathbf{L}$ is associated an observable $\boldsymbol{\mathcal{L}}$ with in turn a corresponding operator $\hat{\boldsymbol{\mathcal{L}}}$. Note that elementary particles have an *intrinsic* angular momentum referred to as spin, next to their *orbital* angular momentum. While the latter has a classical equivalent, the angular momentum $\mathbf{L}$, the former does not. We have seen in *Section* 2.2 that orbital angular momentum is quantised, and it turns out that spin angular momentum also is, see [13][(xxi)]. To begin with, consider a particle without spin. The goal is to obtain operators $\hat{\mathcal{L}}_x, \hat{\mathcal{L}}_y, \hat{\mathcal{L}}_z$ that are associated with the components of orbital angular momentum of the spinless particle. For this we use the fact that an operator $\hat{\mathcal{Q}}$ which describes a classically defined quantity Q is obtained by replacing, in the 'suitably symmetrized' expression for Q, $\mathbf{r}$ and $\mathbf{p}$ by the operators $\hat{\mathbf{R}}$ and $\hat{\mathbf{P}}$ [9]. (Note that generally any physical quantity Q can be expressed in terms of $\mathbf{r}$ and $\mathbf{p}$ only.) To see what a 'suitably symmetrized' expression entails, suppose $Q(\mathbf{r}, \mathbf{p}, t)$ contains a term $\mathbf{r} \cdot \mathbf{p}$. Here, $(\cdot)$ denotes the dot product, which is commutative and so the term can be written as $\mathbf{p} \cdot \mathbf{r}$ instead. However, by the canonical commutation relations the operators $\hat{\mathbf{R}}$ and $\hat{\mathbf{P}}$ (corresponding to the associated observables $\mathbf{R}$ and $\mathbf{P}$) do *not* commute: $[\hat{R}_i, \hat{P}_j] = i\hbar\delta_i^j$, see *Equation* (2.21). That is to say $\hat{\mathbf{R}} \cdot \hat{\mathbf{P}} \neq \hat{\mathbf{P}} \cdot \hat{\mathbf{R}}$. Also $\hat{\mathbf{R}} \cdot \hat{\mathbf{P}}$ and $\hat{\mathbf{P}} \cdot \hat{\mathbf{R}}$ are non-Hermitian [9]. We must hence introduce a symmetrisation rule, which for $\mathbf{r} \cdot \mathbf{p}$ is $(1/2)(\hat{\mathbf{R}} \cdot \hat{\mathbf{P}} + \hat{\mathbf{P}} \cdot \hat{\mathbf{R}})$. Note that this expression is Hermitian as desired.

The x-component of classical angular momentum is given by $\mathbf{L}_x = yp_z - zp_y$, for which we now need to find a suitably symmetrised expression. Associated to y and z are $\hat{R}_y$ and $\hat{R}_z$, respectively, and moreover to p_z and p_y are associated $\hat{P}_z$ and $\hat{P}_y$, respectively. Fortunately, by the canonical commutation relations, $\hat{R}_y$ and $\hat{P}_z$ commute, as do $\hat{R}_z$ and $\hat{P}_y$, which is why no symmetrisation rule needs to be introduced. The operator $\hat{\mathcal{L}}_x$ is given by

$$\hat{\mathcal{L}}_x = \hat{R}_y \hat{P}_z - \hat{R}_z \hat{P}_y.$$

[(xxi)] The so-called spin quantum number can only take non-negative integers or half-integers values, i.e., $0, \frac{1}{2}, 1, \frac{3}{2}, 2, \ldots$.

Since $\hat{R}_y, \hat{R}_z, \hat{P}_y$, and $\hat{P}_z$ are Hermitian, and moreover by using that $[\hat{R}_y, \hat{P}_z] = [\hat{R}_z, \hat{P}_y] = 0$, we have

$$\begin{aligned}\hat{\mathcal{L}}_x^\dagger &= \left(\hat{R}_y\hat{P}_z - \hat{R}_z\hat{P}_y\right)^\dagger \\ &= \hat{P}_z^\dagger\hat{R}_y^\dagger - \hat{P}_y^\dagger\hat{R}_z^\dagger \\ &= \hat{P}_z\hat{R}_y - \hat{P}_y\hat{R}_z \\ &= \hat{R}_y\hat{P}_z - \hat{R}_z\hat{P}_y \\ &= \hat{\mathcal{L}}_x,\end{aligned}$$

so the operator is Hermitian. Completely analogously, we find $\hat{\mathcal{L}}_y = \hat{R}_z\hat{P}_x - \hat{R}_x\hat{P}_z$ and $\hat{\mathcal{L}}_z = \hat{R}_x\hat{P}_y - \hat{R}_y\hat{P}_x$ (also Hermitian). Therefore,

$$\hat{\boldsymbol{\mathcal{L}}} = \hat{\mathbf{R}} \times \hat{\mathbf{P}}. \tag{2.23}$$

Using yet again the canonical commutation relations given in *Equation* (2.21), it follows that

$$\begin{aligned}\left[\hat{\mathcal{L}}_x, \hat{\mathcal{L}}_y\right] &= \left[\hat{R}_y\hat{P}_z - \hat{R}_z\hat{P}_y, \hat{R}_z\hat{P}_x - \hat{R}_x\hat{P}_z\right] \\ &= \left[\hat{R}_y\hat{P}_z, \hat{R}_z\hat{P}_x\right] + \left[\hat{R}_z\hat{P}_y, \hat{R}_x\hat{P}_z\right] \\ &= \hat{R}_y\left[\hat{P}_z, \hat{R}_z\right]\hat{P}_x + \hat{R}_z\left[\hat{R}_y, \hat{P}_x\right]\hat{P}_z + \left[\hat{R}_y, \hat{R}_z\right]\hat{P}_z\hat{P}_x \\ &\quad + \hat{R}_z\hat{R}_y\left[\hat{P}_z, \hat{P}_x\right] + \hat{R}_z\left[\hat{P}_y, \hat{R}_x\right]\hat{P}_z + \hat{R}_x\left[\hat{R}_z, \hat{P}_z\right]\hat{P}_y \\ &\quad + \left[\hat{R}_z, \hat{R}_x\right]\hat{P}_y\hat{P}_z + \hat{R}_x\hat{R}_z\left[\hat{P}_y, \hat{P}_z\right] \\ &= \hat{R}_y\left[\hat{P}_z, \hat{R}_z\right]\hat{P}_x + \hat{R}_x\left[\hat{R}_z, \hat{P}_z\right]\hat{P}_y \\ &= -i\hbar\hat{R}_y\hat{P}_x + i\hbar\hat{R}_x\hat{P}_y \\ &\boxed{= i\hbar\hat{\mathcal{L}}_z}.\end{aligned} \tag{2.24}$$

In a similar fashion, it can be seen that

$$\left[\hat{\mathcal{L}}_y, \hat{\mathcal{L}}_z\right] = i\hbar\hat{\mathcal{L}}_x \qquad \text{and} \qquad \left[\hat{\mathcal{L}}_z, \hat{\mathcal{L}}_x\right] = i\hbar\hat{\mathcal{L}}_y. \tag{2.25}$$

We now introduce a new operator, called the *scalar square of orbital angular momentum*, and it is defined by

$$\hat{\mathcal{L}}^2 := \hat{\mathcal{L}}_x^2 + \hat{\mathcal{L}}_y^2 + \hat{\mathcal{L}}_z^2,$$

which is Hermitian since $\hat{\mathcal{L}}_x, \hat{\mathcal{L}}_y$, and $\hat{\mathcal{L}}_z$ are Hermitian, see above. In fact, corresponding to $\hat{\mathcal{L}}^2$ is the observable $\mathcal{L}^2$ [9]. We claim that $[\hat{\mathcal{L}}^2, \hat{\boldsymbol{\mathcal{L}}}] = 0$. Indeed,

for $\hat{\mathcal{L}}_x$ we have

$$\begin{aligned}\left[\hat{\mathcal{L}}^2, \hat{\mathcal{L}}_x\right] &= \left[\hat{\mathcal{L}}_x^2 + \hat{\mathcal{L}}_y^2 + \hat{\mathcal{L}}_z^2, \hat{\mathcal{L}}_x\right] \\ &= \left[\hat{\mathcal{L}}_x^2, \hat{\mathcal{L}}_x\right] + \left[\hat{\mathcal{L}}_y^2, \hat{\mathcal{L}}_x\right] + \left[\hat{\mathcal{L}}_z^2, \hat{\mathcal{L}}_x\right] \\ &= \hat{\mathcal{L}}_y \left[\hat{\mathcal{L}}_y, \hat{\mathcal{L}}_x\right] + \left[\hat{\mathcal{L}}_y, \hat{\mathcal{L}}_x\right] \hat{\mathcal{L}}_y \\ &\quad + \hat{\mathcal{L}}_z \left[\hat{\mathcal{L}}_z, \hat{\mathcal{L}}_x\right] + \left[\hat{\mathcal{L}}_z, \hat{\mathcal{L}}_x\right] \hat{\mathcal{L}}_z \\ &= -i\hbar \hat{\mathcal{L}}_y \hat{\mathcal{L}}_z - i\hbar \hat{\mathcal{L}}_z \hat{\mathcal{L}}_y + i\hbar \hat{\mathcal{L}}_z \hat{\mathcal{L}}_y + i\hbar \hat{\mathcal{L}}_y \hat{\mathcal{L}}_z \\ &\boxed{= 0}.\end{aligned}$$

where we used that $\hat{\mathcal{L}}_x$ commutes with itself, and the commutation relations of $\hat{\boldsymbol{\mathcal{L}}}$. Similarly, $[\hat{\mathcal{L}}^2, \hat{\mathcal{L}}_y] = [\hat{\mathcal{L}}^2, \hat{\mathcal{L}}_z] = 0$. We hence conclude that $[\hat{\mathcal{L}}^2, \hat{\boldsymbol{\mathcal{L}}}] = 0$[(xxii)].

The orbital angular momentum in the $\{|\mathbf{r}\rangle\}$ representation is given component wise by

$$\hat{\mathcal{L}}_x = \frac{\hbar}{i}\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right), \qquad \hat{\mathcal{L}}_y = \frac{\hbar}{i}\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right),$$
$$\text{and} \quad \hat{\mathcal{L}}_z = \frac{\hbar}{i}\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right),$$

using *Equations* (2.19) and (2.20). This in turn can be expressed in spherical coordinates (ρ, θ, ϕ), after which we find that

$$\hat{\mathcal{L}}_x = i\hbar\left(\sin\phi\frac{\partial}{\partial\theta} + \frac{\cos\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right), \qquad \hat{\mathcal{L}}_y = i\hbar\left(-\cos\phi\frac{\partial}{\partial\theta} + \frac{\sin\phi}{\tan\theta}\frac{\partial}{\partial\phi}\right),$$
$$\text{and} \quad \hat{\mathcal{L}}_z = \frac{\hbar}{i}\frac{\partial}{\partial\phi}. \tag{2.26}$$

It now becomes clear, after some calculations, that

$$\begin{aligned}\hat{\mathcal{L}}^2 &= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right) \\ &= -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right],\end{aligned} \tag{2.27}$$

where the rewriting on the second line makes for a clear similarity with the differential equation of the spherical harmonics Y_l^m as seen in *Equation* (2.10). Below we will investigate this further.

Definition 2.4.3 (Eigenket, eigenvalue, eigenbasis, and spectrum)**.** Let $\mathcal{H}$ be a Hilbert space, $|\psi\rangle \in \mathcal{H}$ a ket, and $\hat{A} : \mathcal{H} \to \mathcal{H}$ an operator. Then, we say $|\psi\rangle$ is an **eigenket** of $\hat{A}$ with **eigenvalue** $\lambda \in \mathbb{C}$ if

$$\hat{A}\,|\psi\rangle = \lambda\,|\psi\rangle\,.$$

[(xxii)] Abusing notation slightly here, similar to *Equation* (2.22).

The set of all eigenvalues is called the **spectrum** of $\hat{A}$, denoted by $\Lambda_{\hat{A}}$. Finally, the set of kets $\mathscr{E} := \{|\psi_i\rangle\}$ such that each $|\psi_i\rangle$ is an eigenket of $\hat{A}$ and $\mathscr{E}$ is a basis of $\mathcal{H}$, is called an **eigenbasis**.

Two remarks are in place here. First, note that if we consider an eigenket $|\psi\rangle$ of an operator $\hat{A}$ with eigenvalue λ, then $z\,|\psi\rangle$ with $z \in \mathbb{C}$ is also an eigenket of $\hat{A}$ with eigenvalue λ. But by condition (II) that is put on $\mathcal{H}$, $|\psi\rangle$ and $z\,|\psi\rangle$ are the same states, so this does not arise any problems. Secondly, one should note that when taking a measurement of an observable $\mathcal{Q}$, the values that can be obtained are those in the spectrum $\Lambda_{\hat{\mathcal{Q}}}$ where $\hat{\mathcal{Q}}$ is the operator corresponding to the observable $\mathcal{Q}$.

Next are some propositions and theorems where it goes without saying that an observable $\mathcal{Q}$ always has corresponding Hermitian operator denoted by $\hat{\mathcal{Q}}$.

Theorem 2.4.4 (Compatibility theorem)**.** Let A, B be observables. The following statements are equivalent:

1. The observables A and B are *compatible*[(xxiii)];
2. The operators $\hat{A}$ and $\hat{B}$ have the same eigenbasis $\mathscr{E}$;
3. $\left[\hat{A}, \hat{B}\right] = 0$, i.e., the operators $\hat{A}$ and $\hat{B}$ commute.

For details on this theorem, see [37, *Section* 5.3].

Consider the commutation relations of orbital angular momentum, described in *Equations* (2.24) and (2.25). The first statement of the theorem implies that it is not possible to measure the three components of orbital angular momentum simultaneously.

Proposition 2.4.5. Given operators $\hat{A}, \hat{B}$ such that $[\hat{A}, \hat{B}] = 0$, and $|\psi\rangle$ an eigenket of $\hat{A}$. Then, $\hat{B}\,|\psi\rangle$ is also an eigenket of $\hat{A}$ with the same eigenvalue.

Proposition 2.4.6. Let A, B be compatible observables. If $|\psi_1\rangle$ and $|\psi_2\rangle$ are two eigenkets of $\hat{A}$ with different eigenvalues, then $\langle\psi_1 \,|\, \hat{B}\psi_2\rangle = 0$.

Theorem 2.4.7. If two observables A, B are compatible, then it is possible to construct an orthonormal basis of the state space $\mathcal{H}$[(xxiv)] with eigenkets common to $\hat{A}$ and $\hat{B}$.

Definition 2.4.8. The set of observables $\{A, B, C, \dots\}$ is called a **complete set of commuting observables** (CSCO) if:

- the observables $A, B, C, \dots$ are pairwise compatible;
- specifying the eigenvalues of all operators $\hat{A}, \hat{B}, \hat{C}, \dots$ determines a unique common eigenket (up to a multiplicative factor).

[(xxiii)] In other words, when measuring one observable, to then subsequently measure the other and finally the first again, the last and first result is guaranteed to be the same.

[(xxiv)] Recall that $\mathcal{H}$ is subject to constraints (I) and (II) outlined at the beginning of this section.

Recall the Hamiltonian for the hydrogen atom system given in *Equation* (2.18).

Claim. $\{H, \mathcal{L}^2, \mathcal{L}_z\}$ is a CSCO.

The proof will follow soon, but we deem it instructive to first prove that $\{\mathcal{L}^2, \mathcal{L}_z\}$ is *not* a CSCO, so at least a third sufficient observable (indeed, the Hamiltonian) needs to be introduced in order to obtain one. Leaving details aside, it turns out that $\hat{\mathcal{L}}^2$ has spectrum $\Lambda_{\hat{\mathcal{L}}^2} = \{l(l+1)\hbar^2 \mid l \in \frac{1}{2}\mathbb{Z}\}$[(xxv)], while $\hat{\mathcal{L}}_z$, for fixed l, has spectrum $\Lambda_{\hat{\mathcal{L}}_z} = \{m_l\hbar \mid m_l \in \{-l, -l+1, \dots, l-1, l\}\}$, see [9]. Using *Equations* (2.26) and (2.27), the eigenkets associated with the eigenvalues of $\hat{\mathcal{L}}_z$ and $\hat{\mathcal{L}}^2$ are respectively the solutions of the partial differential equations

$$\begin{cases} -i\dfrac{\partial}{\partial\phi}\psi(\rho,\theta,\phi) = m\psi(\rho,\theta,\phi), \\ -\left[\dfrac{1}{\sin\theta}\dfrac{\partial}{\partial\theta}\left(\sin\theta\dfrac{\partial}{\partial\theta}\right) + \dfrac{1}{\sin^2\theta}\dfrac{\partial^2}{\partial\phi^2}\right]\psi(\rho,\theta,\phi) = l(l+1)\psi(\rho,\theta,\phi). \end{cases} \tag{2.28}$$

Since ρ is not present in either operators acting on $|\psi(\rho,\theta,\phi)\rangle$, it is considered to be a parameter, allowing us to exclusively consider the θ- and ϕ-dependence of $|\psi\rangle$ [9]. In that case we have, and can confirm by looking at *Equation* (2.10), that for eigenvalues in the spectra $\Lambda_{\hat{\mathcal{L}}^2}$ and $\Lambda_{\hat{\mathcal{L}}_z}$ a common eigenket, which we shall call eigenfunction in this context, of $\hat{\mathcal{L}}^2$ and $\hat{\mathcal{L}}_z$ is the spherical harmonic $Y_l^m(\theta,\phi)$. That is,

$$\hat{\mathcal{L}}^2 Y_l^m(\theta,\phi) = l(l+1)\hbar^2 Y_l^m(\theta,\phi) \qquad \text{and} \qquad \hat{\mathcal{L}}_z Y_l^m(\theta,\phi) = m\hbar Y_l^m(\theta,\phi).$$

Notice that these equations only provide us the θ- and ϕ- dependence of the eigenfunctions of $\hat{\mathcal{L}}^2$ and $\hat{\mathcal{L}}_z$. The eigenfunction depending also on ρ is of the form

$$\psi(\rho,\theta,\phi) = f(\rho)Y_l^m(\theta,\phi).$$

(For the sake of the argument being given, it is on purpose that we do not use $R(\rho)$.) Here, $f(\rho)$ is an integration constant for *Equation* (2.28). That is to say, $f(\rho)$ is, with some regulatory conditions, picked arbitrarily. That means (2) of *Definition* 2.4.8 is not satisfied and hence $\{\hat{\mathcal{L}}^2, \hat{\mathcal{L}}_z\}$ is not a CSCO[(xxvi)].

We now prove the claim that $\{H, \mathcal{L}^2, \mathcal{L}_z\}$ *is* a CSCO.

Proof. In order to see that $[\hat{H}, \hat{\boldsymbol{\mathcal{L}}}] = 0$ (and hence $[\hat{H}, \hat{\mathcal{L}}_z] = 0$) and $[\hat{H}, \hat{\mathcal{L}}_z] = 0$, we rewrite $\hat{H}$ using spherical coordinates (ρ,θ,ϕ). Recall that ∇^2 was given in

[(xxv)] Here, $\frac{1}{2}\mathbb{Z} = \{\dots, -1, -\frac{1}{2}, 0, \frac{1}{2}, 1, \dots\}$ denotes the set of integers and half-integers.

[(xxvi)] If $\mathcal{H} = L^2(\mathbb{S}^2)$ where $\mathbb{S}^2$ is the unit 2-sphere, then $\{\hat{\mathcal{L}}^2, \hat{\mathcal{L}}_z\}$ would be a CSCO, but we are working with $\mathcal{H} = L^2(\mathbb{R}^3)$ here.

Equation (2.7), which can be rewritten:

$$\begin{aligned}\nabla^2 &= \frac{1}{\rho^2}\frac{\partial}{\partial\rho}\left(\rho^2\frac{\partial}{\partial\rho}\right) + \frac{1}{\rho^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\rho^2\sin^2\theta}\left(\frac{\partial^2}{\partial\phi^2}\right)\\ &= \frac{1}{\rho}\frac{\partial^2}{\partial\rho^2}\rho + \frac{1}{\rho^2}\underbrace{\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]}_{=-\hat{\mathcal{L}}^2/\hbar^2}\\ &= \frac{1}{\rho}\frac{\partial^2}{\partial\rho^2}\rho - \frac{1}{\hbar^2\rho^2}\hat{\mathcal{L}}^2,\end{aligned}$$

using the expression for $\hat{\mathcal{L}}^2$ in spherical coordinates given in *Equation* (2.27). Therefore,

$$\begin{aligned}\hat{H} &= -\frac{\hbar^2}{2\mu}\left(\frac{1}{\rho}\frac{\partial^2}{\partial\rho^2}\rho - \frac{1}{\hbar^2\rho^2}\hat{\mathcal{L}}^2\right) + V(\rho)\\ &= -\frac{\hbar^2}{2\mu}\frac{1}{\rho}\frac{\partial^2}{\partial\rho^2}\rho + \frac{1}{2\mu\rho^2}\hat{\mathcal{L}}^2 + V(\rho),\end{aligned}$$

where $V(\rho)$ is the Kepler potential in spherical coordinates, which is not of importance at this moment. By *Equation* (2.26), the components of $\hat{\boldsymbol{\mathcal{L}}}$ act only on θ and ϕ. This implies that these components commute with operators that act only on ρ. Moreover, it has been established that $\hat{\boldsymbol{\mathcal{L}}}$ commutes with $\hat{\mathcal{L}}^2$. Hence it is concluded that $[\hat{H}, \hat{\boldsymbol{\mathcal{L}}}] = 0$. Similarly, $\hat{\mathcal{L}}^2$ also acts only on θ and ϕ, and commutes with itself, so $[\hat{H}, \hat{\mathcal{L}}^2] = 0$ as well. We conclude that $\{H, \mathcal{L}^2, \mathcal{L}_z\}$ is a CSCO. □

Going forward, to make notation less cumbersome, we let $k := e^2/(4\pi\varepsilon_0)$ and choose units such that $m_e = 1$. Also, note that $\hat{\mathbf{P}} = (\hbar)/(i)\nabla$, so we let $\hat{\mathbf{P}}^2 := (\hbar^2)/(i^2)\nabla^2 = -\hbar^2\nabla^2$, and therefore obtain

$$\hat{H} = \frac{\hat{\mathbf{P}}^2}{2} - \frac{k}{r}. \tag{2.29}$$

Besides the angular momentum, we have seen in *Chapter* 1 that the Laplace-Runge-Lenz vector $\mathbf{A}$ also is of importance. Recall that classically $\mathbf{A} = \mathbf{p}\times\mathbf{L} - k\mathbf{r}/r$[(xxvii)], cf. *Definition* 1.3.1. Since $[\hat{\mathcal{L}}_i, \hat{P}_j] \neq 0$ for $i, j \in \{1, 2, 3\}$, it follows that a symmetrisation rule for $\mathbf{p}\times\mathbf{L}$ is needed in obtaining the associated quantum mechanical operator $\hat{\boldsymbol{\mathcal{A}}}$. Consider, analogously to the result in case of the dot product, the symmetrisation rule $(1/2)(\hat{\mathbf{P}}\times\hat{\boldsymbol{\mathcal{L}}} - \hat{\boldsymbol{\mathcal{L}}}\times\hat{\mathbf{P}})$ after which is becomes clear that $\hat{\boldsymbol{\mathcal{A}}}$ can be defined component wise, as follows:

$$\hat{\mathcal{A}}_i\psi(\mathbf{r}) = \frac{1}{2}\left[\left(\hat{\mathbf{P}}\times\hat{\boldsymbol{\mathcal{L}}}\right)_i - \left(\hat{\boldsymbol{\mathcal{L}}}\times\hat{\mathbf{P}}\right)_i\right]\psi(\mathbf{r}) - \frac{k}{r}\hat{R}_i\psi(\mathbf{r}), \tag{2.30}$$

where $i \in \{1, 2, 3\}$. Note that $\psi(\mathbf{r})$ is an arbitrary wave function in the $\{|\mathbf{r}\rangle\}$ representation with $|\psi\rangle \in \mathcal{H}$.

[(xxvii)] Note that we have chosen units such that the $m_e = 1$, hence we omit the μ from *Definition* 1.3.1 here to avoid confusion.

Before continuing, we first develop some notation that will aid us in formulating commutation relations of $\hat{\boldsymbol{\mathcal{L}}}$ and $\hat{\boldsymbol{\mathcal{A}}}$. We shall use the Levi-Civita symbol ε_{ijk} when working with commutators where $i, j, k \in \{1, 2, 3\}$. The symbol can take values $0, 1$, and -1 depending on i, j, and k[(xxviii)]. For $\mathbf{a} = \mathbf{b} \times \mathbf{c}$, we have [24]

$$a_i = \sum_{j=1}^{3} \sum_{k=1}^{3} \varepsilon_{ijk} b_j c_k =: \varepsilon_{ijk} b_j c_k.$$

(Notice the use of compact notation where the summation sign is omitted.) The Levi-Civita symbol is related to the Kronecker delta in the sense that $\varepsilon_{ijk}\varepsilon_{ilm} = \delta^l_j \delta^m_k - \delta^m_j \delta^l_k$ [16].

Theorem 2.4.9. Let $j, k, l \in \{1, 2, 3\}$. The Hamiltonian operator $\hat{H}$ commutes with $\hat{\mathcal{L}}^2$ and the components of $\hat{\boldsymbol{\mathcal{L}}}$ and $\hat{\boldsymbol{\mathcal{A}}}$. That is,

$$\left[\hat{H}, \hat{\mathcal{L}}^2\right] = 0, \qquad \left[\hat{H}, \hat{\mathcal{L}}_i\right] = 0, \qquad \text{and} \qquad \left[\hat{H}, \hat{\mathcal{A}}_i\right] = 0.$$

Moreover, we have the following commutation relations:

$$\begin{aligned}
\left[\hat{R}_j, \hat{\mathcal{L}}_k\right] &= i\hbar\varepsilon_{jkl}\hat{R}_l \qquad & \left[\hat{P}_j, \hat{\mathcal{L}}_k\right] &= i\hbar\varepsilon_{jkl}\hat{P}_l, \\
\left[\hat{\mathcal{L}}_j, \hat{\mathcal{L}}_k\right] &= i\hbar\varepsilon_{jkl}\hat{\mathcal{L}}_l \qquad & \left[\hat{\mathcal{L}}_j, \hat{\mathcal{A}}_k\right] &= i\hbar\varepsilon_{jkl}\hat{\mathcal{A}}_l, \\
\left[\hat{\mathcal{A}}_j, \hat{\mathcal{A}}_k\right] &= -2\hat{H}i\hbar\varepsilon_{jkl}\hat{\mathcal{L}}_l.
\end{aligned}$$

Proof. This is a matter of computation. See [24, 48]. □

At this point, although not entirely obvious, we note that these commutation relations are quite promising. There are various operators commuting with the Hamiltonian, which is directly related to the dynamics of a system through Schrödinger's equation. On the other hand, we have various operators that show strikingly similar commutation relations. This forms a motivation to further investigate these operators and their relations in the following chapters.

[(xxviii)] The Levi-Civita symbol is defined as

$$\varepsilon_{ijk} := \begin{cases} +1 & \text{if } (i,j,k) \text{ is } (1,2,3),\ (2,3,1), \text{ or } (3,1,2), \\ -1 & \text{if } (i,j,k) \text{ is } (3,2,1),\ (1,3,2), \text{ or } (2,1,3), \\ 0 & \text{if } i = j,\ j = k, \text{ or } k = i. \end{cases}$$

So, $\varepsilon_{ijk} = 1$ when (i, j, k) is an even permutation of $(1, 2, 3)$ while $\varepsilon_{ijk} = -1$ when it is odd. If an index is repeated we have $\varepsilon_{ijk} = 0$. For more details and properties we refer to [4].

Chapter 3

(Hidden) Symmetry of the Hydrogen Atom

In the previous chapter, it was seen that the commutator plays a crucial role in quantum mechanics, but moreover it was seen that they are of special importance in our study on the hydrogen atom because of the specific commutation relations. The aim of this chapter is to set up a framework of Lie groups and Lie algebras, named after the Norwegian mathematician Sophus Lie, and use this this in describing symmetries. We follow the thought of Singer [39] throughout this chapter.

The reader is assumed to be familiar with groups.

3.1 Lie Groups

Before delving into the concept of Lie groups, we briefly review what manifolds are. One can consider many types of manifolds: topological, analytic, complex, but also $\mathscr{C}^\infty$-manifolds[(xxix)]. The latter will be of interest to us. In textbooks such as [27, 46] one starts with topological manifolds and transfer ideas of calculus to them, thereby arriving at $\mathscr{C}^\infty$-manifolds. These are then spaces that in a local sense 'look like' $\mathbb{R}^n$, moreover admitting calculus. Examples of $\mathscr{C}^\infty$-manifolds include $\mathbb{R}^n$, finite-dimensional vector spaces, and spaces of matrices [27].

We can now specify how a Lie group is defined.

Definition 3.1.1 (Lie group)**.** A group G with group operations m and ι is said to be a **Lie group** if it is a $\mathscr{C}^\infty$-manifold such that $m, \iota \in \mathscr{C}^\infty$ where $m : G \times G \to G$ and $\iota : G \to G$, the multiplication and inverse map, respectively, are given by [27]

$$m : (g, h) \mapsto gh \qquad \text{and} \qquad \iota : g \mapsto g^{-1}.$$

Notice that a Lie group possesses both a group and a manifold structure. Below we consider some examples of Lie groups, namely $SO(n)$ and $SU(2)$.

[(xxix)] By $\mathscr{C}^\infty$ we denote infinitely differentiable. A $\mathscr{C}^\infty$-manifold is also called a smooth manifold.

Definition 3.1.2 ($SO(n)$ groups)**.** The **special orthogonal group** $SO(n)$ where $n \in \mathbb{Z}_{>0}$ is defined as [43]

$$SO(n) := \{M \in GL(\mathbb{R}^n) \mid M^T M = I, \det M = 1\}.$$

Note that $GL(\mathcal{V})$ denotes the set of invertible linear transformations from $\mathcal{V}$ to itself, where $\mathcal{V}$ is any vector space[(xxx)]. For example, $SO(3)$ is the group of rotations of the Euclidean space $\mathbb{R}^3$. Notice that rotations are linear transformations and hence $SO(3)$ can be described as a group of matrices using the standard basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\} := \{(1,0,0)^T, (0,1,0)^T, (0,0,1)^T\}$. Introducing some notation, we say $R_{\hat{\mathbf{u}}}(\theta) \in SO(3)$ is a rotation about a unit vector $\hat{\mathbf{u}}$ with angle θ in the positive direction. Using the standard basis, rotations about the coordinate axes are given by [47]

$$R_{\mathbf{e_1}}(\theta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}, \qquad R_{\mathbf{e_2}}(\theta) = \begin{bmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{bmatrix},$$
$$\text{and} \quad R_{\mathbf{e_3}}(\theta) = \begin{bmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{bmatrix}. \tag{3.1}$$

Now, the group $SO(3)$ can be explicitly parametrised using the commonly used Euler angles ϕ, θ, and ψ. The idea behind this parametrisation is that a general rotation is expressed as a rotation about the z-axis by ϕ, subsequently performing a rotation about the newly obtained x-axis by θ, to finally rotate around the new z-axis by ψ. That is, a general rotation is expressed as $R(\phi, \theta, \psi)$ defined by

$$R(\phi, \theta, \psi) = R_{\mathbf{e_3}}(\psi) R_{\mathbf{e_1}}(\theta) R_{\mathbf{e_3}}(\phi).$$

Also see *Figure* 3.1 below. The group $SO(3)$ will be used extensively throughout the text, since it inherently is of concern as the natural representation of $SO(3)$ on $L^2(\mathbb{R}^3)$ models the electron in the hydrogen atom.

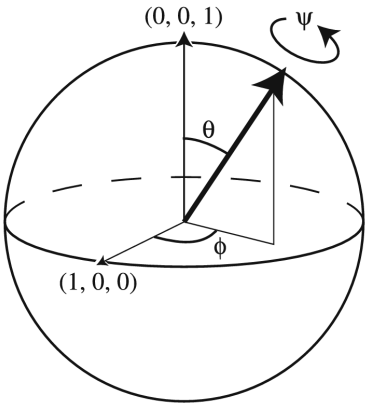

Figure 3.1: Euler angles. Taken from [39].

[(xxx)] This vector space $\mathcal{V}$ is taken over a field. We note, first of all, that $GL(\mathcal{V})$ is a group where the binary operation is composition of transformations. Upon choosing a basis for $\mathcal{V}$, one can write $M \in GL(\mathcal{V}$ as a matrix. See [39] for more details.

Another example of a Lie group is $SU(2)$, defined by

$$SU(2) := \{M \in GL\left(\mathbb{C}^2\right) \mid M^\dagger M = I,\, \det M = 1\}.$$

Definition 3.1.3 (Lie group homomorphism and isomorphism)**.** Let G and H be Lie groups, and $\varphi : G \to H$ a group homomorphism. If $\varphi \in \mathscr{C}^\infty$, then φ is a **Lie group homomorphism**. Moreover, if φ is also a group isomorphism and $\varphi^{-1} \in \mathscr{C}^\infty$, then φ is a **Lie group isomorphism**.

Definition 3.1.4 (Representation)**.** Consider a (Lie) group G, vector space $\mathcal{V}$, and (Lie) group homomorphism $\varphi : G \to GL(\mathcal{V})$. Then, the triple $(G, \mathcal{V}, \varphi)$ is a **(Lie group) representation** of G on $\mathcal{V}$.

The set of all invertible transformations from a set $\mathcal{S}$ to itself it denoted by $\mathcal{T}(\mathcal{S}, \mathcal{S})$ and forms a group under composition of transformations.

Definition 3.1.5 (Action)**.** Let G be a group, $\mathcal{S}$ a set, and $\sigma : G \to \mathcal{T}(\mathcal{S}, \mathcal{S})$ a group homomorphism. An **action**[(xxxi)] of G on S is a triple $(G, \mathcal{S}, \sigma)$.

Every representation is an action, but not necessarily the other way around. For example, consider the action $(\mathbb{R}, \mathbb{R}, \sigma)$ of the group $\mathbb{R}$ on the real line $\mathbb{R}$, with the 'multiplication' map of the group being addition, i.e., $m : (x, y) \mapsto x + y$. We define $\sigma : \mathbb{R} \to \mathcal{T}(\mathbb{R}, \mathbb{R})$ as $t \mapsto \sigma(t)$ where the transformation $\sigma(t) : \mathbb{R} \to \mathbb{R}$ is given by $x \mapsto x + t$. Notice that $\sigma(t)$ is a *linear* transformation if and only if $t = 0$, and therefore it is seen that although $(\mathbb{R}, \mathbb{R}, \sigma)$ is an action, it is not a representation. Now, if we have an action $(G, \mathcal{S}, \sigma)$, there exists a representation $(G, \mathcal{V}, \rho)$ where $\mathcal{V}$ is the complex vector space of complex-valued functions on $\mathcal{S}$, and ρ is given by [39]

$$\begin{aligned} \rho(g) \cdot f : \mathcal{S} &\to \mathcal{V} \\ s &\mapsto f\left(\sigma\left(g^{-1}\right) s\right), \end{aligned}$$

for each $g \in G$ and $f \in \mathcal{V}$. In this way, the representation $(G, \mathcal{V}, \rho)$ corresponds to the action $(G, \mathcal{S}, \sigma)$.

Definition 3.1.6 (Unitary operator, group, and representation)**.** Suppose $\mathcal{H} := L^2(\mathbb{R}^n)$.

1. The operator $\hat{U}$ on $\mathcal{H}$ is said to be a **unitary operator** if

$$\hat{U}^\dagger \hat{U} = \hat{U}\hat{U}^\dagger = \hat{I},$$

   where $\hat{I}$ denotes the identity operator on $\mathcal{H}$.

2. The **unitary group**[(xxxii)] of $\mathcal{H}$ is denoted by $\mathcal{U}(\mathcal{H})$ and is the group of unitary operators on $\mathcal{H}$.

[(xxxi)] There are left actions and right actions. We restrict to left actions only. Hence, given an action we automatically speak about a left action.

[(xxxii)] Unitary operators indeed form a group since the composition of two unitary operators on $\mathcal{H}$ is unitary, and moreover every unitary operator on $\mathcal{H}$ has an inverse unitary operator on $\mathcal{H}$.

3. A (Lie group) representation $(G, \mathcal{H}, \rho)$ is a **unitary representation** if the image of ρ lies in $\mathcal{U}(\mathcal{H})$.

We make the assumption that all representations being considered in a quantum mechanical setting are unitary. Moreover, for our purposes, when discussing representations we say that they are always Lie group representations, because we will be working solely with Lie groups and Lie group homomorphisms.

Notice that by the above definition, one can conclude that unitary operators preserve length and angles between vectors. Consider a hydrogen atom with state space $\mathcal{H} = L^2(\mathbb{R}^3)$. We shall consider the *natural representation* of $SO(3)$ on $\mathcal{H}$. Note first that since $SO(3)$ is the group of rotations in $\mathbb{R}^3$, we find a natural action of $SO(3)$ on $\mathbb{R}^3$. Therefore a natural representation of $SO(3)$ on the $\mathcal{H}$ must exist. Indeed, after 'rotating a square-integrable function' we acquire again a square-integrable function. Explicitly, for the natural representation of $SO(3)$ on $\mathcal{H}$, we have for any $R \in SO(3)$ and any $|\psi\rangle \in \mathcal{H}$ the function $R \cdot |\psi\rangle$, defined by

$$(R \cdot |\psi\rangle)(\mathbf{r}) := |\psi\rangle \left(R^{-1}\mathbf{r}\right),$$

where $\mathbf{r} \in \mathbb{R}^3$. We now look at how a representation of $SO(3)$ on $\mathcal{H}$ is obtained by considering different observers positioned equidistantly from a hydrogen atom. In order to find such a representation $(G, \mathcal{H}, \varphi)$ we need to find a group homomorphism $\varphi : SO(3) \to GL(\mathcal{H})$. To that end, consider the sphere of *Figure* 3.2 below with two observers A and B such that if a fixed rotation $g \in SO(3)$ is applied on the sphere, the new location and facing of A is the old location and facing of B. We say that the position of the observers differ by g.

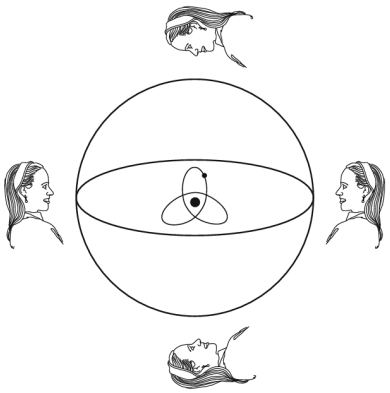

Figure 3.2: Hydrogen atom symmetry

The task now is to find the linear transformation $\varphi_g : \mathcal{H} \ni |\psi_1\rangle \mapsto |\psi_2\rangle \in \mathcal{H}$. Suppose observer A describes the hydrogen atom as being in state $|\psi_1\rangle \in \mathcal{H}$, and similarly observer B finds the hydrogen atom in state $|\psi_2\rangle \in \mathcal{H}$, then we define $\varphi_g |\psi_1\rangle := |\psi_2\rangle$. That is, $\varphi_g |\psi_1\rangle \in \mathcal{H}$ is the state that observer B would find the hydrogen atom in given that A finds it in $|\psi_1\rangle$. This definition for φ_g is independent of observers A and B, as choosing observers A', B' that also differ by g yields the same φ_g. It can be readily seen that φ_g is a linear transformation, i.e., that

$$\varphi_g(\lambda |\psi_1\rangle + \mu |\psi_1\rangle) = \lambda \varphi_g |\psi_1\rangle + \mu \varphi_g |\psi_2\rangle .$$

For the particular details we refer to [39]. We claim that $\varphi := \varphi_g$ is a group homomorphism. Indeed, when we have three observers A, B and C, and if A, B di□er by g while B, C di□er by h, then A, C di□er by hg. Then $\varphi_{hg} : \mathcal{H} \to \mathcal{H}$ is a linear transformation where state vectors in the perspective of A are mapped to state vectors in the perspective of C. However, this is exactly the same as mapping a state vector in the perspective of A to a state vector in the perspective of B, and then mapping the latter vector to a state vector in the perspective of C, so we find that $\varphi_{hg} = \varphi_h \varphi_g$.

By assumption, but which can also be verified, $(SO(3), \mathcal{H}, \varphi)$ is a *unitary* representation. It is also assumed that φ is a Lie group homomorphism, and therefore that $\varphi \in \mathscr{C}^\infty$. The latter can be seen experimentally as observed data changes smoothly as an observer changes position smoothly [39].

What can be concluded here, is that the symmetry group of the hydrogen atom contains $SO(3)$ as a subgroup. In *Section* 1.4, we discussed the concept of hidden symmetry. In the current setting, this corresponds to showing that $SO(4)$, the group of rotations in $\mathbb{R}^4$, is *also* contained as a subgroup of the symmetry group of the hydrogen atom. This will be the considered further in *Chapter* 4. Some theory that will be required for this chapter will be developed in the following section. First, we state some definitions for further reference. Here we assume G is a (Lie) group.

Definition 3.1.7 (Invariant subspace)**.** Consider a representation $(G, \mathcal{V}, \varphi)$. A subspace $\mathcal{W}$ of $\mathcal{V}$ is called an **invariant subspace** of $(G, \mathcal{V}, \varphi)$ if $g \cdot w \in \mathcal{W}$ for all $g \in G$ and $w \in \mathcal{W}$.

Definition 3.1.8 (Irreducible representation)**.** A representation $(G, \mathcal{V}, \varphi)$ is an **irreducible representation** if its only invariant subspaces are $\mathcal{V}$ and the zero subspace $\{\mathbf{0}\}$. Moreover, we say a representation is *reducible* if it is not irreducible.

Definition 3.1.9 (Homomorphism/isomorphism of representations)**.** Let $(G, \mathcal{V}, \rho)$ and $(G, \mathcal{W}, \tilde{\rho})$ be representations, and $T : \mathcal{V} \to \mathcal{W}$ a linear transformation. Then, T is called a **homomorphism of representations** $(G, \mathcal{V}, \rho)$ and $(G, \mathcal{W}, \tilde{\rho})$ if

$$\tilde{\rho}(g) \circ T = T \circ \rho(g)$$

for all $g \in G$.

3.2 Homogeneous Harmonic Polynomials

Consider the vector space of polynomials in three real variables with complex coe□cients, denoted by $\mathscr{P}_3$.

Definition 3.2.1 (Harmonic polynomial)**.** Let $p \in \mathscr{P}_3$ be a polynomial. We say p is **harmonic** if

$$\nabla^2 p = 0,$$

where ∇^2 is the Laplacian. The set of all harmonic polynomials of $\mathscr{P}_3$ is denoted by $\mathbb{H}$. That is,

$$\mathbb{H} := \{p \in \mathscr{P}_3 \mid \nabla^2 p = 0\}.$$

Note that $\mathbb{H}$ forms a subspace of $\mathscr{P}_3$. We shall prove this statement. It follows from the definition of $\mathbb{H}$ that it is a subset of $\mathscr{P}_3$. Now, let $p_1, p_2 \in \mathbb{H}$ and $\lambda \in \mathbb{C}$. We need to show that $\lambda p_1 + p_2 \in \mathbb{H}$. Indeed,

$$\begin{aligned} \nabla^2(\lambda p_1 + p_2) &= \nabla^2(cp_1) + \nabla^2 p_2 && \nabla^2 \text{ is distributive} \\ &= \lambda \nabla^2 p_1 + \nabla^2 p_2 && \lambda \text{ is constant} \\ &= 0, && p_1, p_2 \text{ are harmonic,} \end{aligned}$$

for all $p_1, p_2 \in \mathbb{H}$ and $\lambda \in \mathbb{C}$. Therefore $\lambda p_1 + p_2 \in \mathbb{H}$ as desired, and hence it is concluded that $\mathbb{H}$ is a subspace of $\mathscr{P}_3$.

Definition 3.2.2 (Homogeneous polynomial)**.** Let $f = \sum_{i=0}^{n} a_i x_1^{d_{i_1}} x_2^{d_{i_2}} \cdots x_k^{d_{i_k}}$ be a polynomial with coe□cients $a_i \in \mathbb{C}$, $i \in \{0, 1, \ldots, n\}$, and variables $x_1, x_2, \ldots, x_k \in \mathbb{C}$, where $d_{i_j} \in \mathbb{Z}_{\geq 0}$ is the degree in x_j, $j \in \{1, 2, \ldots, k\}$, for the ith term. Then, the degree of the ith term is

$$d_i = d_{i_1} + d_{i_2} + \cdots + d_{i_k}.$$

If $d_1 = d_2 = \cdots = d_n =: d$, then the polynomial f is said to be a **homogeneous polynomial** of degree d.

Consider the homogeneous polynomials of degree n in two variables $x, y \in \mathbb{R}$, with coe□cients in $\mathbb{C}$[(xxxiii)]. These polynomials form a complex vector space, which we shall denote by $\mathscr{P}_2^n$. The basis of $\mathscr{P}_2^n$ is of the form

$$\left\{x^n, x^{n-1}y, x^{n-2}y^2, \ldots, x^2y^{n-2}, xy^{n-1}, y^n\right\},$$

and consists of $n+1$ elements, and therefore the dimension of $\mathscr{P}_2^n$ is $n+1$. Similarly, the homogeneous complex-valued polynomials of degree l in three variables also form a complex vector space, denoted by $\mathscr{P}_3^l$, and has dimension $(l+1)(l+2)/2$. For details on this claim, see [39, *Section* 2.2].

Definition 3.2.3 ($\mathbb{H}^l$ and $\mathscr{Y}^l$)**.** Let $l \in \mathbb{Z}_{\geq 0}$. The vector space of **homogeneous harmonic polynomials** of degree l in three variables is defined by

$$\mathbb{H}^l := \{p \in \mathscr{P}_3^l \mid \nabla^2 p = 0\}.$$

The restricted polynomials of $\mathbb{H}^l$ to the 2-sphere $\mathbb{S}^2$ is also a vector space, given by

$$\mathscr{Y}^l := \left\{p|_{\mathbb{S}^2} \mid p \in \mathbb{H}^l\right\}.$$

Proposition 3.2.4. Let $l \in \mathbb{Z}_{\geq 0}$. Then,

$$\operatorname{span}\{Y_l^m \mid m \in \{-l, \ldots, -1, 0, 1, \ldots, l\}\} = \mathscr{Y}^l,$$

where Y_l^m are the spherical harmonics, see *Equation* (2.13).

Proof. We provide merely a sketch of the proof. For further details we refer to [39, *Proposition* A.2]. In proving that the spherical harmonics indeed span $\mathscr{Y}^l$,

[(xxxiii)] We say that the polynomial is *complex-valued*.

we first show that

$$\{Y_l^m\} := \{Y_l^m \mid m \in \{-l, \ldots, -1, 0, 1, \ldots, l\}\}$$

is linearly independent, which can be achieved by considering an arbitrary linear combination equal to zero. Suppose

$$\sum_{m=-l}^{l} C_m \exp(im\phi) P_l^m(\cos\theta) = 0,$$

then one can show that $C_m = 0$ for all allowed m. Furthermore it can be shown that $\{Y_l^m\} \subset \mathscr{Y}^l$. We now combine the previous two statements. Notice that there are $2l+1$ possible values of m. It follows by the linear independence of $\{Y_l^m\}$ and the fact that $\{Y_l^m\} \subset \mathscr{Y}^l$, that the spherical harmonics Y_l^m span a $(2l+1)$-dimensional subset of $\mathscr{Y}^l$. Since $\dim \mathscr{Y}^l \leq 2l+1$, we find that $\operatorname{span}\{Y_l^m\} = \mathscr{Y}^l$ as desired. □

Because of the relation with the spherical harmonics when restricting a polynomial $p \in \mathbb{H}^l$ to the 2-sphere $\mathbb{S}^2$, consider the following.

The natural representation of $SO(3)$ on $L^2(\mathbb{S}^2)$ is given explicitly by

$$(g \cdot f)(\mathbf{x}) = f(g^{-1}\mathbf{x}),$$

where $g \in SO(3)$, $f \in L^2(\mathbb{S}^2)$, and $\mathbf{x} \in \mathbb{S}^2$.

Proposition 3.2.5. Let $l \in \mathbb{Z}_{\geq 0}$, and consider the natural representation of $SO(3)$ on $L^2(\mathbb{S}^2)$. Then, the subspace $\mathscr{Y}^l$ of $L^2(\mathbb{S}^2)$ is invariant.

Proof. It needs to be shown that $g \cdot y \in \mathscr{Y}^l$ for all $g \in SO(3)$ and $y \in \mathscr{Y}^l$. To that end, let $g \in SO(3)$ and $y \in \mathscr{Y}^l$. Using *Definition* 3.2.3, it follows that there exists $p \in \mathbb{H}^l$ such that $y = p|_{\mathbb{S}^2}$. After rotating p, it will still be of the same degree l showing that $g \cdot p$ is a homogeneous polynomial of degree l. Moreover, $\nabla^2 p = 0$ since the Laplacian is invariant under rotation as it is a homomorphism of representations. This then shows that $g \cdot p$ is harmonic. Therefore $g \cdot p \in \mathbb{H}^l$ after which it can be concluded that $g \cdot y = g|_{\mathbb{S}^2} \cdot p \in \mathscr{Y}^l$. □

For the proofs of the propositions below, we refer to [39, *Chapter* 7].

Proposition 3.2.6. Let $l \in \mathbb{Z}_{\geq 0}$, and $\mathbb{H}^l$ the vector space of homogeneous harmonic polynomials of degree l in three variables. We have that $\dim \mathbb{H}^l = 2l+1$.

Proposition 3.2.7. Let $l \in \mathbb{Z}_{\geq 0}$. The natural representation of $SO(3)$ on $\mathbb{H}^l$ is irreducible.

3.3 Lie Algebras

In *Definition* 3.1.1, it was seen that a Lie group G possesses a group structure, as well as a manifold structure. It turns out that locally, the group G looks the same around any point. Crucial information about the Lie group is concentrated

in a small neighbourhood of the identity element e [46]. It is therefore natural to consider the tangent space at the identity, which we denote as T_eG.

Before continuing we explain how a tangent space should be thought of. In the space $\mathbb{R}^n$, we can at any point p define a tangent vector describing, in physical terms, the velocity at that point. The tangent space is then the set of tangent vectors at the point p, which can be viewed as a vector space describing all possible velocities at that point. The idea of tangent vectors and spaces generalises in a manifold M. However, we often adopt a more abstract way of viewing a tangent vector where it would be seen as a linear map called a *derivation*, obeying Leibniz's di□erentiation rule. In some sense, this is more fruitful as one has now obtained a more versatile setting to work in, such as the possibility of composing with other maps. When a manifold is embedded in a space $\mathbb{R}^n$, for some $n \in \mathbb{Z}_{>0}$, that is, the space surrounding the manifold is $\mathbb{R}^n$, then the tangent space stretches a hyperplane touching the manifold 'tangentially' at a certain point.

The tangent space T_eG is a vector space that we can equip with a bracket $[\cdot, \cdot]$. We then arrive at the definition of what we call a Lie algebra, see below. We are interested in proving the presence of $SO(4)$-symmetry in the quantum Kepler problem. However, since Lie algebras encode information about Lie groups, such as $SO(4)$, and moreover there indeed *is* a Lie algebra associated to $SO(4)$, we pursue looking at structures on the Lie algebra level.

Definition 3.3.1 (Real Lie algebra)**.** A **real Lie algebra** is a real vector space $\mathfrak{g}$ with bracket[(xxxiv)] $[\cdot, \cdot] : \mathfrak{g} \times \mathfrak{g} \to \mathfrak{g}$ satisfying

1. Asymmetry: $[A, B] = -[B, A]$;
2. Bilinearity: $[\lambda A + \mu B, C] = \lambda[A, C] + \mu[B, C]$ and $[A, \lambda B + \mu C] = \lambda[A, B] + \mu[A, C]$;
3. Jacobi identity: $[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$,

for all $A, B, C \in \mathfrak{g}$ and $\lambda, \mu \in \mathbb{R}$.

An example of a Lie algebra the set of $n \times n$ matrices with complex entries, which is denoted by $\mathfrak{gl}(n, \mathbb{C})$[(xxxv)] and has commutator $[A, B] := AB - BA$ where $A, B \in \mathfrak{gl}(n, \mathbb{C})$. Notice the similarity between the commutator of $\mathfrak{gl}(n, \mathbb{C})$ and the commutator of operators in *Definition* 2.4.1.

We described that a Lie algebra is the tangent space at the identity element equipped with a commutator. To more explicitly relate the Lie group to its Lie algebra, we focus on cases where the Lie group is a group consisting of matrices as we can then define the Lie algebra concretely. Consider the Lie group $SO(n)$ defined in *Definition* 3.1.2. Then, the Lie algebra $\mathfrak{so}(n)$ of $SO(n)$ is the space of $n \times n$ matrices A such that $\exp(tA) \in SO(n)$, where $t \in \mathbb{R}$ [47]. We note

(xxxiv) Throughout this text, we refer to the bracket $[\cdot, \cdot]$ as the *commutator* because of the connection of the commutator as defined in *Definition* 2.4.1.

(xxxv) This naturally is a complex vector space, however, one can think of it as a real Lie algebra. See [39, *Section* 8.1].

that the exponential of a matrix A of size $n \times n$ is given by

$$e^A := \sum_{k=0}^{\infty} \frac{1}{k!} A^k = I_{n\times n} + A + \frac{1}{2!}A^2 + \frac{1}{3!}A^3 + \cdots + \frac{1}{n!}A^n + \cdots ,$$

i.e. a power series[(xxxvi)]. To fully understand what $\mathfrak{so}(n)$ looks like, consider the following claim.

Claim. Let

$$A = \begin{bmatrix} 0 & -\theta \\ \theta & 0 \end{bmatrix}.$$

Then, $\exp A$ is a rotation matrix given by

$$\exp A = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}.$$

Proof. We follow the thought of [17, *Chapter* 14]. First note that

$$A = \theta \underbrace{\begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix}}_{=:X} \quad \text{and} \quad A^2 = -\theta^2 \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = -\theta^2 I_{2\times 2}.$$

Using these expression, it can be established that

$$\begin{aligned} A^{4k} &= \theta^{4k} I_{2\times 2} & A^{4k+1} &= \theta^{4k+1} X \\ A^{4k+2} &= -\theta^{4k+2} I_{2\times 2} & A^{4k+3} &= -\theta^{4k+3} X. \end{aligned}$$

Therefore,

$$\begin{aligned} e^A &= \sum_{k=0}^{\infty} \frac{1}{k!} A^k \\ &= I_{2\times 2} + \theta X - \frac{\theta^2}{2!} I_{2\times 2} - \frac{\theta^3}{3!} X + \frac{\theta^4}{4!} I_{2\times 2} + \frac{\theta^5}{5!} X - \cdots \\ &= \underbrace{\left(1 - \frac{\theta^2}{2!} + \frac{\theta^4}{4!} - \cdots\right)}_{=\cos\theta} I_{2\times 2} + \underbrace{\left(\theta - \frac{\theta^3}{3!} + \frac{\theta^5}{5!} - \cdots\right)}_{=\sin\theta} X \\ &= \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}, \end{aligned}$$

using the power series for $\cos\theta$ and $\sin\theta$. □

The above can be generalised. That is, for a *anti-symmetric* matrix A of size $n \times n$ (such as the one from the claim), then $\exp A$ is a matrix where $AA^T = I_{n\times n}$ and $\det A = 1$. Conversely, every rotation matrix is of this form. We hence arrive at the definition of the Lie algebra $\mathfrak{so}(n)$ associated to $SO(n)$:

$$\mathfrak{so}(n) := \{A \in \mathfrak{gl}(n, \mathbb{R}) \mid A + A^T = 0\}.$$

[(xxxvi)] The power series is convergent for any matrix A.

That is, the Lie algebra of $\mathfrak{so}(n)$ consists of real $n \times n$ matrices that are anti-symmetric[(xxxvii)]. We can also give the fundamental relation between $\mathfrak{so}(n)$ and $SO(n)$, namely, the map

$$\exp : \mathfrak{so}(n) \to SO(n),$$

which is a well-defined and surjective [17].

Matrices in $\mathfrak{so}(n)$ correspond to elements in the tangent space at the identity of $SO(n)$. These matrices also correspond to *infinitesimal rotations*. The definition below will make this statement clear. Here, we use Rodrigues' formula, which we shall state first.

Proposition 3.3.2 (Rodrigues' formula)**.** Let $\mathbf{u}$ be a unit vector. A rotation through an angle θ about the direction along $\mathbf{u}$ is given by [17]:

$$R_{\mathbf{u}}(\theta) = I_{n\times n} + (\sin\theta)G_{\mathbf{u}} + (1-\cos\theta)G_{\mathbf{u}}^2,$$

where $G_{\mathbf{u}} \in \mathfrak{so}(n)$[(xxxviii)].

When we take the angle to be very small, $|\theta| \ll 1$, we find that $\sin\theta \approx \theta$, while $1-\cos\theta \approx 0$. Using Taylor expansions to the first order, we have the following definition.

Definition 3.3.3 (Infinitesimal rotation and generator)**.** Let $\mathbf{u}$ be a unit vector. An **infinitesimal rotation** is a rotation through an infinitesimally small angle $|\mathrm{d}\theta| \ll 1$ about the direction along $\mathbf{u}$, and it given by [6]

$$R_{\mathbf{u}}(\mathrm{d}\theta) = I_{n\times n} + \mathrm{d}\theta G_{\mathbf{u}} + \mathcal{O}(\mathrm{d}\theta^2).$$

Here, $G_{\mathbf{u}} \in \mathfrak{so}(n)$ is called the **generator** of the infinitesimal rotation.

We now look at what these generator matrices look like for the Lie algebra $\mathfrak{so}(3)$. Consider the standard basis $\{\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3\}$. In *Equation* (3.1), we saw the matrices for three-dimensional rotations. For example, when rotating about the vector $\mathbf{e}_1$ by an angle θ in the positive direction, we have

$$R_{\mathbf{e}_1}(\theta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{bmatrix}.$$

The corresponding infinitesimal rotation matrix is

$$R_{\mathbf{e}_1}(\mathrm{d}\theta) = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & -\mathrm{d}\theta \\ 0 & \mathrm{d}\theta & 1 \end{bmatrix} + \mathcal{O}(\mathrm{d}\theta^2) = I_{3\times 3} + \mathrm{d}\theta \underbrace{\begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}}_{=:G_1} + \mathcal{O}(\mathrm{d}\theta^2).$$

[(xxxvii)] The anti-symmetric property corresponds to the requirement $A + A^T = 0$ where $A \in \mathfrak{so}(n)$. Note that we therefore have $\mathrm{Tr}\, A = 0$.

[(xxxviii)] This matrix is further attended to shortly.

In a similar manner, we find $R_{\mathbf{e}_2}(\mathrm{d}\theta) = I_{3\times 3} + \mathrm{d}\theta G_2 + \mathcal{O}(\mathrm{d}\theta^2)$ and $R_{\mathbf{e}_3}(\mathrm{d}\theta) = I_{3\times 3} + \mathrm{d}\theta G_3 + \mathcal{O}(\mathrm{d}\theta^2)$[xxxix], where

$$G_2 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix} \quad \text{and} \quad G_3 = \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix}.$$

We call G_1, G_2, and G_3 the infinitesimal rotation generators of $\mathfrak{so}(3)$. They satisfy the commutation relations

$$[G_j, G_k] = \varepsilon_{jkl} G_l. \tag{3.2}$$

A Lie algebra can have a *Lie subalgebra*. If we have a vector subspace $\mathfrak{h}$ of some Lie algebra $\mathfrak{g}$, then $\mathfrak{h}$ is also a Lie algebra if $[A, B] \in \mathfrak{h}$ for all $A, B \in \mathfrak{h}$. The Lie algebra $\mathfrak{h}$ inherits its structure from $\mathfrak{g}$, and so we say that $\mathfrak{h}$ is a Lie subalgebra of $\mathfrak{g}$. A Lie subalgebra of $\mathfrak{gl}(2, \mathbb{C})$ is the special unitary algebra, defined as

$$\mathfrak{su}(2) := \{A \in \mathfrak{gl}(2, \mathbb{C}) \mid A + A^\dagger = 0,\ \mathrm{Tr}\, A = 0\},$$

where $\mathrm{Tr}\, A$ is the *trace* of the matrix $A \in \mathfrak{gl}(n, \mathbb{C})$, defined by the sum of its diagonal entries. Since $A \in \mathfrak{su}(2)$ satisfy $A = -A^\dagger$, we say A is *anti-Hermitian*, cf. *Definition* 2.4.2. Note that elements of $\mathfrak{su}(2)$ are of the form

$$\begin{bmatrix} iX & Y + iZ \\ -Y + iZ & -iX \end{bmatrix},$$

where $X, Y, Z \in \mathbb{R}$. We shall make an e□ort to describe a basis for $\mathfrak{su}(2)$ which proves to be helpful later in this section.

Claim. A basis for $\mathfrak{su}(2)$:

$$\{B_1, B_2, B_3\} := \left\{ \frac{1}{2}\begin{bmatrix} i & 0 \\ 0 & -i \end{bmatrix}, \frac{1}{2}\begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}, \frac{1}{2}\begin{bmatrix} 0 & i \\ i & 0 \end{bmatrix} \right\}. \tag{3.3}$$

Proof. See [39, 47]. □

Definition 3.3.4 (Lie algebra homomorphism/isomorphism)**.** Let $\mathfrak{g}_1$ and $\mathfrak{g}_2$ be Lie algebras with commutators $[\,\cdot\,,\,\cdot\,]_1$ and $[\,\cdot\,,\,\cdot\,]_2$, respectively. Also let $T : \mathfrak{g}_1 \to \mathfrak{g}_2$ be a linear transformation.

- We say T is a **Lie algebra homomorphism** if

  $$[TA, TB]_2 = T\left([A, B]_1\right),$$

  for all $A, B \in \mathfrak{g}_1$.

- If T is bijective, then T is called a **Lie algebra isomorphism**, which can be expressed as $\mathfrak{g}_1 \cong \mathfrak{g}_2$.

[xxxix] Instead of rotating about one of the basis vectors $\mathbf{e}_1, \mathbf{e}_2$, or $\mathbf{e}_3$, we also say that we rotate about the corresponding axis.

To define a Lie algebra homomorphism $T : \mathfrak{g}_1 \to \mathfrak{g}_2$, it suffices to define it on basis elements of $\mathfrak{g}_1$, and check that the commutation relations are satisfied [39, *Chapter* 8]. This can be seen by realising that once the basis elements are specified, they uniquely define T as this map is linear. Moreover, if the basis elements satisfy $[TA, TB]_2 = T([A, B]_1)$, where $A, B \in \mathfrak{g}_1$ and the commutators are of the respective Lie algebras $\mathfrak{g}_1$ and $\mathfrak{g}_2$, then an arbitrary linear combination of basis elements will also satisfy this equality.

We often drop the index of the commutator when it is clear from the context what commutator is at hand.

Claim. $\mathfrak{su}(2) \cong \mathfrak{so}(3)$.

Proof. Consider the basis

$$\{G_1, G_2, G_3\} := \left\{ \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{bmatrix}, \begin{bmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{bmatrix}, \begin{bmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} \right\} \tag{3.4}$$

for $\mathfrak{so}(3)$. On the other hand, recall the basis $\{B_1, B_2, B_3\}$ for $\mathfrak{su}(2)$ presented in *Equation* (3.3). Let $i \in \{1, 2, 3\}$. The map $T : \mathfrak{so}(3) \to \mathfrak{su}(2)$ where $G_i \mapsto B_i$ is bijective, and moreover the commutator satisfies

$$[B_j, B_k] = \varepsilon_{jkl} B_l.$$

This can be verified by checking with different indices. We provide an example:

$$[TG_1, TG_2] = [B_1, B_2] = B_3 = TG_3 = T[G_1, G_2].$$

The point is that the commutation relations are the same as the ones for G_i, see *Equation* (3.2). It is therefore concluded that $\mathfrak{su}(2) \cong \mathfrak{so}(3)$. □

Definition 3.3.5 (Cartesian sum)**.** Let $\mathfrak{g}_1$ and $\mathfrak{g}_2$ be Lie algebras with commutators $[\cdot, \cdot]_1$ and $[\cdot, \cdot]_2$, respectively. The **Cartesian sum** $\mathfrak{g}_1 \oplus \mathfrak{g}_2$ is a Lie algebra with commutator

$$[(A_1, A_2), (B_1, B_2)] := ([A_1, B_1]_1, [A_2, B_2]_2),$$

for all $A_1, A_2 \in \mathfrak{g}_1$ and $B_1, B_2 \in \mathfrak{g}_2$.

Claim. $\mathfrak{so}(3) \oplus \mathfrak{so}(3) \cong \mathfrak{so}(4)$.

Proof. We first construct a basis for the Lie algebra $\mathfrak{so}(4)$. Consider a four-dimensional space with coordinate axes x, y, z, and w. Three of the generators of $\mathfrak{so}(4)$ are obtained by fixing the w-plane and considering rotations about the left-over axis x, y, and z using the basis $\{G_1, G_2, G_3\}$ for $\mathfrak{so}(3)$ G_i previously found, see *Equation* (3.4). That is,

$$J_i = \begin{bmatrix} & & & 0 \\ & G_i & & 0 \\ & & & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix},$$

where $i \in \{1,2,3\}$ are three out of six generators of $\mathfrak{so}(4)$. The other three generators of $\mathfrak{so}(4)$ correspond to rotations in the xw-, yw-, and zw-plane. Those are

$$\tilde{J}_1 = \begin{bmatrix} & & & -1 \\ & 0_{3\times 3} & & 0 \\ & & & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, \quad \tilde{J}_2 = \begin{bmatrix} & & & 0 \\ & 0_{3\times 3} & & -1 \\ & & & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix},$$

$$\text{and,} \quad \tilde{J}_3 = \begin{bmatrix} & & & 0 \\ & 0_{3\times 3} & & 0 \\ & & & -1 \\ 0 & 0 & 1 & 0 \end{bmatrix},$$

respectively. A basis for $\mathfrak{so}(4)$ then consists of all previously mentioned generators of $\mathfrak{so}(4)$:

$$\{J_1, J_2, J_3, \tilde{J}_1, \tilde{J}_2, \tilde{J}_3\}.$$

Of interest are their commutation relations. One can verify that

$$[J_j, J_k] = \varepsilon_{jkl} J_l, \quad [\tilde{J}_j, \tilde{J}_k] = \varepsilon_{jkl} J_l, \quad \text{and,} \quad [J_j, \tilde{J}_k] = \varepsilon_{jkl} \tilde{J}_l.$$

The generators J_1, J_2, J_3 satisfy the same commutation relations as those of $\mathfrak{so}(3)$. The latter were described in *Equation* (3.2). In light of the claim, we expect that the generators $\tilde{J}_1, \tilde{J}_2, \tilde{J}_3$ also satisfy the commutation relations of $\mathfrak{so}(3)$. This is however not self-evident at this point. So we define

$$K_i := \frac{1}{2}(J_i + \tilde{J}_i) \quad \text{and} \quad M_i := \frac{1}{2}(J_i - \tilde{J}_i),$$

where $i \in \{1,2,3\}$. We then have

$$[K_j, K_k] = \varepsilon_{jkl} K_l, \quad [M_j, M_k] = \varepsilon_{jkl} M_l, \quad \text{and,} \quad [K_j, M_k] = 0. \tag{3.5}$$

This now shows that K_1, K_2, K_3 satisfy the commutation relations of $\mathfrak{so}(3)$, and so do M_1, M_2, M_3. It is concluded that $\mathfrak{so}(4)$ is a Cartesian sum of two Lie algebras $\mathfrak{so}(3)$, i.e.

$$\mathfrak{so}(3) \oplus \mathfrak{so}(3) \cong \mathfrak{so}(4),$$

as desired. □

Since we already established that $\mathfrak{su}(2) \cong \mathfrak{so}(3)$, one might notice that indeed $\mathfrak{su}(2) \oplus \mathfrak{su}(2) \cong \mathfrak{so}(4)$.

In the remainder of this section, we will show that rescaled linear combinations of the Laplace-Runge-Lenz operator and angular momentum operator yield the same commutation relations as *Equation* (3.5). Recall the Laplace-Runge-Lenz operator $\hat{\boldsymbol{\mathcal{A}}}$, defined component wise in *Equation* (2.30), and the angular momentum operator $\hat{\boldsymbol{\mathcal{L}}}$. It was concluded in *Theorem* 2.4.9 that we

have the following commutation relations related to $\hat{\boldsymbol{\mathcal{A}}}$ and $\hat{\boldsymbol{\mathcal{L}}}$:

$$\left[\hat{\mathcal{L}}_j, \hat{\mathcal{L}}_k\right] = i\hbar\varepsilon_{jkl}\hat{\mathcal{L}}_l \qquad \left[\hat{\mathcal{L}}_j, \hat{\mathcal{A}}_k\right] = i\hbar\varepsilon_{jkl}\hat{\mathcal{A}}_l,$$
$$\left[\hat{\mathcal{A}}_j, \hat{\mathcal{A}}_k\right] = -2i\hbar\varepsilon_{jkl}\hat{H}\hat{\mathcal{L}}_l.$$

using the Levi-Civita symbol ε_{jkl}. Let

$$\hat{K}_j := \frac{1}{2i\hbar}\left(\sqrt{-\frac{1}{2E}}\hat{\mathcal{A}}_j + \hat{\mathcal{L}}_j\right) \quad \text{and} \quad \hat{M}_j := \frac{1}{2i\hbar}\left(\sqrt{-\frac{1}{2E}}\hat{\mathcal{A}}_j - \hat{\mathcal{L}}_j\right),$$

where $j \in \{1, 2, 3\}$. Now, by using the bilinearity property of the commutator, we have

$$\begin{aligned}
\left[\hat{K}_1, \hat{K}_2\right] &= \left[\frac{1}{2i\hbar}\left(\sqrt{-\frac{1}{2E}}\hat{\mathcal{A}}_1 + \hat{\mathcal{L}}_1\right), \frac{1}{2i\hbar}\left(\sqrt{-\frac{1}{2E}}\hat{\mathcal{A}}_2 + \hat{\mathcal{L}}_2\right)\right] \\
&= \frac{1}{2i\hbar}\sqrt{-\frac{1}{2E}}\left(\frac{1}{2i\hbar}\sqrt{-\frac{1}{2E}}\left[\hat{\mathcal{A}}_1, \hat{\mathcal{A}}_2\right] + \frac{1}{2i\hbar}\left[\hat{\mathcal{A}}_1, \hat{\mathcal{L}}_2\right]\right) \\
&\quad + \frac{1}{2i\hbar}\left(\frac{1}{2i\hbar}\sqrt{-\frac{1}{2E}}\left[\hat{\mathcal{L}}_1, \hat{\mathcal{A}}_2\right] + \frac{1}{2i\hbar}\left[\hat{\mathcal{L}}_1, \hat{\mathcal{L}}_2\right]\right) \\
&= \frac{1}{4}\left(\frac{1}{i\hbar}\right)^2\left(-\frac{1}{2E}\left[\hat{\mathcal{A}}_1, \hat{\mathcal{A}}_2\right]\right. \\
&\quad \left. + \sqrt{-\frac{1}{2E}}\left(\left[\hat{\mathcal{A}}_1, \hat{\mathcal{L}}_2\right] + \left[\hat{\mathcal{L}}_1, \hat{\mathcal{A}}_2\right]\right) + \left[\hat{\mathcal{L}}_1, \hat{\mathcal{L}}_2\right]\right).
\end{aligned}$$

Now, $[\hat{\mathcal{A}}_1, \hat{\mathcal{A}}_2] = -2i\hbar\hat{H}\hat{\mathcal{L}}_3$ and since $\hat{H}\,|\psi\rangle = E\,|\psi\rangle$, we have, after consulting the commutation relations, that

$$-\frac{1}{2E}\left[\hat{\mathcal{A}}_1, \hat{\mathcal{A}}_2\right] = -\frac{-2i\hbar E}{2E}\hat{\mathcal{L}}_3 = i\hbar\hat{\mathcal{L}}_3.$$

Moreover, $[\hat{\mathcal{A}}_1, \hat{\mathcal{L}}_2] = -[\hat{\mathcal{L}}_2, \hat{\mathcal{A}}_1] = -i\hbar(-1)\hat{\mathcal{A}}_3 = i\hbar\hat{\mathcal{A}}_3$, $[\hat{\mathcal{L}}_1, \hat{\mathcal{A}}_2] = i\hbar\hat{\mathcal{A}}_3$, and $[\hat{\mathcal{L}}_1, \hat{\mathcal{L}}_2] = i\hbar\hat{\mathcal{L}}_3$ are also obtained by considering the respective commutation relation. Therefore,

$$\begin{aligned}
\left[\hat{K}_1, \hat{K}_2\right] &= \frac{1}{4}\left(\frac{1}{i\hbar}\right)^2\left(2i\hbar\hat{\mathcal{L}}_3 + 2i\hbar\sqrt{-\frac{1}{2E}}\hat{\mathcal{A}}_3\right) \\
&= \frac{1}{2i\hbar}\left(\sqrt{-\frac{1}{2E}}\hat{\mathcal{A}}_3 + \hat{\mathcal{L}}_3\right) \\
&\boxed{= \hat{K}_3}.
\end{aligned}$$

By performing similar computations, one concludes that

$$\left[\hat{K}_j, \hat{K}_k\right] = \varepsilon_{jkl}\hat{K}_l.$$

Moreover, by some more effort where one keeps a close track on sign changes, it is found that

$$\left[\hat{M}_j, \hat{M}_k\right] = \varepsilon_{jkl}\hat{M}_l \quad \text{and} \quad \left[\hat{K}_j, \hat{M}_k\right] = 0.$$

These commutation relations are precisely the ones of *Equation* (3.5). That is, both $\hat{K}_j$ and $\hat{M}_j$ satisfy the commutation relations of $\mathfrak{so}(3)$, where $j \in \{1, 2, 3\}$. Therefore taking the operators $\hat{K}_i$ together with $\hat{M}_i$, we have a Lie algebra $\mathfrak{so}(4)$ structure. We do not exactly speak of $\mathfrak{so}(4)$-symmetry at this point because, as seen in *Section* 1.4, for symmetry we need to have invariance of *dynamics* under certain transformations. However, the dynamics of a quantum system are subject to the wave function which is in turn governed by the Schrödinger equation where the Hamiltonian operator $\hat{H}$ plays a central role. Therefore, the fact that $\hat{\boldsymbol{\mathcal{L}}}$ and $\hat{\boldsymbol{\mathcal{A}}}$ commute with the Hamiltonian operator $\hat{H}$, allows us to say that the hydrogen atom system, which models the quantum Kepler problem, shows $\mathfrak{so}(4)$-symmetry.

In the next chapter, the goal is to generalise things substantially. The desire is to show that the Lie *group* $SO(4)$ is a symmetry group of the quantum Kepler problem. However, the generalisations go further than this, in the sense that we let the main focus rest on hidden symmetry in the quantum Kepler problem of arbitrary dimension. We use different techniques than in this chapter.

Chapter 4

Hidden Symmetry of the Quantum Kepler Problem in n Dimensions

To summarise our work up to this point, we have described the classical Kepler problem where three-dimensional rotational symmetry was found. Relatively unexpectedly, one could also find four-dimensional rotational symmetry, hence speaking of hidden symmetry. In the quantum mechanical picture, which is in a sense more fundamental, we established the same with a slight catch. That is, we only obtained symmetry in the Lie *algebra* $\mathfrak{so}(4)$. As remarked in [39], $SO(4)$-symmetry is in a sense no better than $\mathfrak{so}(4)$-symmetry, since some important properties of the hydrogen atom can be concluded from both symmetries. Recall that Lie algebras contains information about its corresponding Lie group. The $\mathfrak{so}(4)$-symmetry is hence on its own impressive and should not be written o□. Yet, we want to pave a road towards 'full' $SO(4)$-symmetry. This is what Vladimir Fock managed to show in his article '*Zur Theorie des Wassersto atoms*' ('On the Theory of the Hydrogen Atom') [15] published in 1935. An English translation is provided in [39, *Chapter* 9]. The argument relies on two cornerstones: a method of interchanging position and momentum representations, and the application of a stereographic projection. These will be elaborated on in the *Sections* 4.2 and 4.3, respectively.

One might wonder, given $SO(4)$ symmetry of the hydrogen atom , what happens when we consider the quantum Kepler problem in an arbitrary dimension n? It is not self-evident whether hidden symmetry can be found in that case. To answer the question, we examine the argument by Bander and Itzykson in [2]. They elaborate on the generalisation of Fock's method to any dimension. The goal of this chapter is to lay out the generalisation process. Moreover, we solve the quantum Kepler problem in the sense of obtaining the spectrum of the Hamiltonian operator. We note that in 1926 it was Wolfgang Pauli who was able to first describe the spectrum of the hydrogen atom in a bound state, see [35].

Before delving into the matter, we have some preliminaries that need to be discussed.

4.1 Preliminary Notions

First of all, we note that the n-sphere $\mathbb{S}^n$ is constructed by taking all $\mathbf{x} \in \mathbb{R}^{n+1}$ such that their distance from the origin is one, where we consider the Euclidean

norm for the distance. In other words,

$$\mathbb{S}^n := \left\{ \mathbf{x} \in \mathbb{R}^{n+1} \mid x = 1 \right\}.$$

Recall *Definition* 3.2.3 where we considered the vector space of complex-valued polynomials of degree l in three variables, denoted by $\mathscr{P}_3^l$. Analogous to that, we denote by $\mathscr{P}_{n+1}^l$ the vector space of homogeneous complex-valued polynomials of degree l in $n+1$ variables. We moreover have some analogies presented in the following definition.

Definition 4.1.1 ($\mathbb{H}_{n+1}^l$ and $\mathscr{Y}_{n+1}^l$)**.** Let $l \in \mathbb{Z}_{\geq 0}$. The vector space of **homogeneous harmonic polynomials** of degree l in $n+1$ variables is defined by

$$\mathbb{H}_{n+1}^l := \{ p \in \mathscr{P}_{n+1}^l \mid \nabla^2 p = 0 \}.$$

The restricted polynomials of $\mathbb{H}_{n+1}^l$ to the n-sphere $\mathbb{S}^n$ is also a vector space, given by

$$\mathscr{Y}_{n+1}^l := \left\{ p|_{\mathbb{S}^n} \mid p \in \mathbb{H}_{n+1}^l \right\}.$$

Let $h \in \mathbb{H}_{n+1}^l$, that is, p is a homogenous harmonic polynomial of degree l in $n+1$ variables. Note that h depends on

$$\binom{n+l}{l}$$

coe□cients. Moreover, since h is harmonic, i.e. $\nabla^2 h = 0$, note that there are

$$\binom{n+l-2}{l-2}$$

homogeneous boundary conditions. So, the number of independent h with degree l is

$$\binom{n+l}{l} - \binom{n+l-2}{l-2} = \frac{(n+2l-1)(n+l-2)!}{(n-1)!l!}.$$

We therefore arrive at the following proposition.

Proposition 4.1.2. Let $l \in \mathbb{Z}_{\geq 0}$. We have

$$\dim \mathscr{P}_{n+1}^l = \frac{(n+l)!}{n!l!},$$

and

$$\dim \mathbb{H}_{n+1}^l = \frac{(n+2l-1)(n+l-2)!}{(n-1)!l!}. \tag{4.1}$$

The propositions that follows will prove to be beneficial in our later analysis.

Proposition 4.1.3. Let $l \in \mathbb{Z}_{\geq 0}$ and $p \in \mathscr{P}_{n+1}^l$[(xl)]. Then,

$$\sum_{i=1}^{n+1} x_i \frac{\partial}{\partial x_i} p = lp. \tag{4.2}$$

[(xl)] That is, a homogeneous polynomial of degree l in $n+1$ variables. Recall that hence p is complex-valued. It has complex coe□cients, and real variables.

Proposition 4.1.4. The Laplacian on $\mathbb{R}^n$, denoted by $\nabla_{\mathbb{R}^n}$, is given by

$$\nabla^2_{\mathbb{R}^n} = \sum_{j=1}^{n} \frac{\partial^2}{\partial x_j^2}$$

in Cartesian coordinates. Moreover, in spherical coordinates, we have

$$\nabla^2_{\mathbb{R}^n} = \frac{\partial^2}{\partial r^2} + \frac{n-1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Delta_{\mathbb{S}^n}.$$

Proposition 4.1.5 (Green's second identity)**.** Let $u, w \in \mathscr{C}^k$[(xli)] where $k \geq 2$ on some region $D \subset \mathbb{R}^n$. We then have [5]

$$\int_D \left(u\nabla^2 w - w\nabla^2 u\right) \mathrm{d}v = \oint_{\partial D} \left(u\frac{\partial w}{\partial \boldsymbol{\nu}} - w\frac{\partial u}{\partial \boldsymbol{\nu}}\right) \mathrm{d}s, \tag{4.3}$$

where ∂D is the boundary of the region D, and $\boldsymbol{\nu}$ is outward pointing surface normal of the surface element $\mathrm{d}s$.

4.2 The Fourier Transform

A crucial element in the generalisation process is the formulation of Schrödinger's equation

$$\hat{H}\left|\psi\right\rangle = E\left|\psi\right\rangle,$$

in n dimensions. The Hamiltonian operator $\hat{H}$ we are concerned with is easily obtained by generalising *Equation* (2.2), as described below that equation, and the Kepler potential given in *Equation* (2.16). We find that

$$\hat{H} = -\frac{\hbar^2}{2\mu}\nabla^2_{\mathbb{R}^n} - \frac{k}{r}.$$

Therefore, in the $\{|\mathbf{r}\rangle\}$ representation, Schrödinger's equation for the Kepler potential, which we shall call the *Kepler-Schrödinger equation*, becomes

$$\left(-\frac{\hbar^2}{2\mu}\nabla^2_{\mathbb{R}^n} - \frac{k}{r}\right)\left|\psi(\mathbf{r})\right\rangle = E\left|\psi(\mathbf{r})\right\rangle. \tag{4.4}$$

In large part, the aim of Fock [15], and subsequently Bander and Itzykson [2] where Fock's argument is generalised, is solving this equation. In order to do so, the equation is transformed to momentum space, that is, obtaining it in the $\{|\mathbf{p}\rangle\}$ representation. This is done with the use of a Fourier transform[(xlii)] [11]:

$$\hat{\psi}(\mathbf{p}) = A_n \int_{\mathbb{R}^n} \psi(\mathbf{r}) \exp\left(-\frac{i\,\mathbf{p}\cdot\mathbf{r}}{\hbar}\right) \mathrm{d}\mathbf{r}.$$

(xli) That is, u and w are at least twice continuously differentiable functions.
(xlii) The hat on ψ refers to the Fourier transform.

Here, A_n is a constant we deliberately do not specify since there are multiple conventions for it, and it will cancel out regardless in our analysis.

Before continuing, consider the following definition.

Definition 4.2.1 (Gamma function)**.** Let $x \in \mathbb{R}_{>0}$. The **gamma function**, denoted by Γ, is given by [8]

$$\Gamma(x) := \int_0^\infty t^{x-1} \exp(-t)\, \mathrm{d}t.$$

We derive a property of the gamma function known as the *functional relationship* that shall be used at a later stage. By using integration by parts, we find

$$\begin{aligned}
\Gamma(x+1) &= \int_0^\infty t^x \exp(-t)\, \mathrm{d}t \\
&= \left[-t^x \exp(-t)\right]_0^\infty + \int_0^\infty x t^{x-1} \exp(-t)\, \mathrm{d}t \\
&= x \int_0^\infty t^{x-1} \exp(-t)\, \mathrm{d}t \\
&= x\Gamma(x), \qquad (4.5)
\end{aligned}$$

where $x \in \mathbb{R}_{>0}$.

Proposition 4.2.2. In the $\{|\mathbf{p}\rangle\}$ representation, the Kepler-Schrödinger equation is given by

$$\frac{1}{2}\left(p^2 - 2\mu E\right) |\hat{\psi}(\mathbf{p})\rangle = C_n \int_{\mathbb{R}^n} \frac{|\hat{\psi}(\mathbf{p}')\rangle}{\|\mathbf{p}-\mathbf{p}'\|^{n-1}}\, \mathrm{d}^n\mathbf{p}', \qquad (4.6)$$

where

$$C_n = \frac{\mu k \Gamma\left(\frac{n-2}{2}\right)}{2\pi^{\frac{n+1}{2}}\hbar}.$$

Here, Γ denotes the gamma function.

Proof. We provide a sketch. For details, see [29, 18]. We denote the Fourier transform of a function f by $\hat{f}$, and the latter is obtained by performing the Fourier transform operator on f, that is, $\mathcal{F}(f) = \hat{f}$. Note that for $\mathbf{r} \in \mathbb{R}^d$ we have

$$\mathcal{F}\left(\frac{1}{r}\right) = \frac{2^{n-1}\pi^{\frac{n-1}{2}}\Gamma\left(\frac{n-1}{2}\right)}{p^{n-1}}.$$

Moreover, since

$$\mathcal{F}(fg) = \frac{1}{(2\pi)^n}\mathcal{F}(f) * \mathcal{F}(g),$$

we have that

$$\mathcal{F}\left(\frac{k}{r}\psi(\mathbf{r})\right) = \frac{1}{(2\pi)^n}\mathcal{F}\left(\frac{1}{r}\right) * \mathcal{F}\left(k\psi(\mathbf{r})\right).$$

□

4.3 Stereographic Projections

Besides Fourier transformations, the argument of Fock also relies on stereographic projections. Recall that the n-sphere $\mathbb{S}^n$ is given by

$$\mathbb{S}^n := \left\{ \mathbf{x} \in \mathbb{R}^{n+1} \mid x = 1 \right\},$$

Note that on $\mathbb{S}^n$ itself, we use the *spherical metric* for distance instead. Given $\mathbf{x}, \mathbf{y} \in \mathbb{S}^n$, the spherical metric, denoted by $d_{\mathbb{S}^n}$, is given by

$$d_{\mathbb{S}^n}(\mathbf{x}, \mathbf{y}) := \arccos\left(\frac{\langle \mathbf{x}, \mathbf{y} \rangle}{xy} \right).$$

That is, the metric $d_{\mathbb{S}^n}$ corresponds to angles in $\mathbb{R}^{n+1}$ between $\mathbf{x}$ and $\mathbf{y}$ using the standard inner product on $\mathbb{R}^{n+1}$. We moreover say that the n-sphere $\mathbb{S}^n$ has both a *north* and a *south* pole, given by $\mathbf{N} = (0, 0, \ldots, 1)$ and $\mathbf{S} = (0, 0, \ldots, -1)$, respectively. The idea behind the stereographic projection is that when we consider an n-sphere where one point is removed, let this point without loss of generality be the north pole, there is a topological equivalence to the space $\mathbb{R}^n$. This will become clear in the following definition.

Definition 4.3.1. Consider an n-sphere $\mathbb{S}^n$. The **stereographic projection** is a function $\sigma : \mathbb{S}^n \setminus \{\mathbf{N}\} \to \mathbb{R}^n$ where

$$\mathbf{X} = (X_1, X_2, \ldots, X_{n+1}) \overset{\sigma}{\mapsto} \frac{(X_1, X_2, \ldots, X_n)}{1 - X_{n+1}}. \tag{4.7}$$

Proposition 4.3.2. The stereographic projection σ of an n-sphere $\mathbb{S}^n$ is bijective. We have that σ^{-1} is given by

$$\mathbf{x} = (x_1, x_2, \ldots, x_n) \overset{\sigma^{-1}}{\mapsto} \frac{(2x_1, 2x_2, \ldots, 2x_n, x^2 - 1)}{x^2 + 1}.$$

4.4 Negative Energies ($E < 0$)

We consider the quantum Kepler problem in a bounded state, that is, where we have negative values for the energy E.

Let $p_0 = \sqrt{-2\mu E}$ and $p_j = p_0 x_j$ where $j \in \{1, \ldots, n\}$. Suppose the n-dimensional space $\mathbb{R}^n$ is embedded with coordinates x_j into a $(n+1)$-dimensional space $\mathbb{R}^{n+1}$ with coordinates X_j.

$$\sigma^{-1} : \mathbb{R}^n \to \mathbb{S}^n \setminus \{\mathbf{N}\}$$
$$\mathbf{x} := (x_1, x_2, \ldots, x_n) \mapsto (X_1, X_2, \ldots, X_{n+1}) =: \mathbf{X},$$

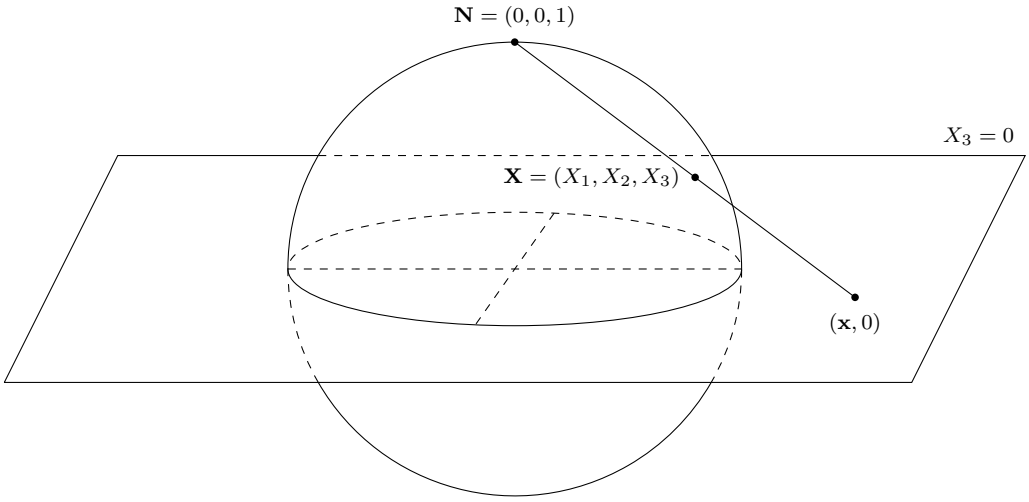

Figure 4.1: In the stereographic projection for the three-dimensional case, we have the mapping $\sigma : \mathbb{S}^3 \setminus \{\mathbf{N}\} \to \mathbb{R}^3$, where $\mathbf{N} = (0, 0, 1)$ is the north pole.

where

$$X_j = \frac{2x_j}{x^2 + 1}, \quad j \in \{1, \dots, n\}$$
$$X_{n+1} = \frac{x^2 + 1}{x^2 - 1}.$$

Note that $x_j = X_j/(1-X_{n+1})$ by *Equation* (4.7), and moreover that $\langle \mathbf{X}, \mathbf{X} \rangle = 1$, so we find

$$\begin{aligned} x^2 &= \frac{1 - X_{n+1}^2}{(1 - X_{n+1})^2} \\ &= \frac{1 + X_{n+1}}{1 - X_{n+1}}. \end{aligned}$$

Now let

$$\Psi(\mathbf{X}) := \frac{1}{\sqrt{p_0}} \left(\frac{p^2 + p_0^2}{2p_0} \right)^{\frac{n+1}{2}} \hat{\psi}(\mathbf{p}).$$

Lemma 4.4.1 (Virial)**.** Whenever $E < 0$, we have that

$$E \int_{\mathbb{R}^n} |\hat{\psi}(\mathbf{p})|^2 \, \mathrm{d}^n\mathbf{p} = -\int_{\mathbb{R}^n} \frac{p^2}{2\mu} |\hat{\psi}(\mathbf{p})|^2 \, \mathrm{d}^n\mathbf{p}.$$

Theorem 4.4.2. The map $\mathscr{L} : \hat{\psi}(\mathbf{p}) \mapsto \Psi(X)$ belonging to a fixed E is a linear isometry[(xliii)].

[(xliii)] That is, $\mathscr{L}$ preserves norms: $\|\mathscr{L}\hat{\psi}\| = \|\hat{\psi}\|$. Since we are working in an inner product space, this is equivalent to $\langle \mathscr{L}\hat{\psi} \,|\, \mathscr{L}\hat{\psi} \rangle = \langle \hat{\psi} \,|\, \hat{\psi} \rangle$, cf. *Definition* 2.1.1.

Proof. It needs to be shown that $\langle \mathscr{L}\hat{\psi} \,|\, \mathscr{L}\hat{\psi}\rangle = \langle \hat{\psi} \,|\, \hat{\psi}\rangle$. To that end,

$$\begin{aligned}\langle \mathscr{L}\hat{\psi} \,|\, \mathscr{L}\hat{\psi}\rangle &= \langle \Psi \,|\, \Psi\rangle \\ &= \int_{\mathbb{S}^n} |\Psi(X)|^2 \,\mathrm{d}\Omega_n \\ &= \int_{\mathbb{R}^n} \frac{p^2 + p_0^2}{2p_0^2} |\hat{\psi}(\mathbf{p})|^2 \,\mathrm{d}^n\mathbf{p} \\ &= \int_{\mathbb{R}^n} \frac{p^2}{2p_0^2} |\hat{\psi}(\mathbf{p})|^2 \,\mathrm{d}^n\mathbf{p} + \int_{\mathbb{R}^n} \frac{1}{2} |\hat{\psi}(\mathbf{p})|^2 \,\mathrm{d}^n\mathbf{p}.\end{aligned}$$

We now use the virial theorem together with the fact that $p_0 = \sqrt{-2\mu E}$. Then, we find

$$\begin{aligned}\langle \mathscr{L}\hat{\psi} \,|\, \mathscr{L}\hat{\psi}\rangle &= \int_{\mathbb{R}^n} \frac{-2\mu E}{2(-2\mu E)} |\hat{\psi}(\mathbf{p})|^2 \,\mathrm{d}^n\mathbf{p} + \int_{\mathbb{R}^n} \frac{1}{2} |\hat{\psi}(\mathbf{p})|^2 \,\mathrm{d}^n\mathbf{p} \\ &= \int_{\mathbb{R}^n} |\hat{\psi}(\mathbf{p})|^2 \,\mathrm{d}^n\mathbf{p} \\ &= \langle \hat{\psi} \,|\, \hat{\psi}\rangle \,,\end{aligned}$$

as desired. □

The map in the previous theorem can be extended to a map

$$\mathscr{T} : \mathcal{H} \to L^2(\mathbb{S}^n), \tag{4.8}$$

where $\mathcal{H}$ is the completion of the pre-Hilbert space of linear combinations of eigenkets corresponding to the negative eigenvalues in $\Sigma_{\hat{H}}$, i.e., the spectrum of the Hamiltonian.

Claim. The eigenkets corresponding to different negative eigenvalues in $\Sigma_{\hat{H}}$ are orthogonal.

Proof. This follows immediately from *Proposition* 2.4.6. □

Moreover, an analogous claim can be made for solutions of *Equation* (4.6) corresponding to different eigenvalues of p_0. Hence the map $\mathscr{T}$ is an injective and unitary[(xliv)] isometry.

Claim. The Kepler-Schrödinger equation given in *Equation* (4.6) is equivalent to

$$C_n \int_{\mathbb{S}^n} \frac{\Psi(\mathbf{X}')}{\|\mathbf{X} - \mathbf{X}'\|^{n-1}} \,\mathrm{d}\Omega'_n = p_0 \Psi(\mathbf{X}), \tag{4.9}$$

where

$$C_n = \frac{\mu k \Gamma\left(\frac{n-2}{2}\right)}{2\pi^{\frac{n+1}{2}}\hbar},$$

[(xliv)] In *Definition* 3.1.6 we define unitary operators. Now, $\mathscr{T}$ is not an operator since it does not map to itself, however, we still say that $\mathscr{T}$ being unitary means $\mathscr{T}^\dagger\mathscr{T} = \mathscr{T}\mathscr{T}^\dagger = I_{\mathcal{H}}$.

and the volume form is given by

$$\mathrm{d}\Omega_n = \left(\frac{2}{x^2+1}\right)^n \mathrm{d}^n\mathbf{x}.$$

Proof. First, note that

$$\begin{aligned}
\|\mathbf{X}-\mathbf{X}'\|^2 &= \langle \mathbf{X}-\mathbf{X}', \mathbf{X}-\mathbf{X}'\rangle \\
&= \langle \mathbf{X},\mathbf{X}\rangle + \langle \mathbf{X}',\mathbf{X}'\rangle - 2\langle \mathbf{X},\mathbf{X}'\rangle \qquad \text{since } \langle \mathbf{X},\mathbf{X}'\rangle \text{ is purely real} \\
&= 2 - 2\frac{4\langle \mathbf{x},\mathbf{x}'\rangle + (x^2-1)((x')^2-1)}{(x^2+1)((x')^2+1)} \\
&= 4\frac{\|\mathbf{x}-\mathbf{x}'\|^2}{(x^2+1)((x')^2+1)}.
\end{aligned}$$

Next, notice that $p_j = p_0 x_j$ and therefore $x_j = p_j/p_0$ where $p_0 = \sqrt{-2\mu E}$ and $j \in \{1,\ldots,n\}$. Hence:

- $X_j = \dfrac{2x_j}{x^2+1} = \dfrac{2}{p^2/p_0^2+1}\dfrac{p_j}{p_0} = \dfrac{2p_0}{p^2-p_0^2}p_j$;
- $X_{n+1} = \dfrac{x^2+1}{x^2-1} = \dfrac{p^2/p_0+1}{p^2/p_0-1} = \dfrac{p^2+p_0^2}{p^2-p_0^2}$;
- $\mathrm{d}\Omega_n = \left(\dfrac{2}{x^2+1}\right)^n \mathrm{d}^n\mathbf{x} = \left(\dfrac{2}{p^2/p_0+1}\right)^n \mathrm{d}^n\dfrac{1}{p_0}\mathbf{p} = \left(\dfrac{2p_0}{p^2-p_0^2}\right)^n \mathrm{d}^n\mathbf{p}$;
- $\|\mathbf{X}-\mathbf{X}'\|^2 = \dfrac{4\|\mathbf{x}-\mathbf{x}'\|^2}{(x^2+1)((x')^2+1)} = \dfrac{4p_0^2\|\mathbf{p}-\mathbf{p}'\|^2}{(p^2-p_0^2)((p')^2-p_0^2)}$,

with $j \in \{1,\ldots,n\}$. After making the substitutions and some rewriting, it becomes clear that

$$C_n \int_{\mathbb{R}^n} \frac{|\hat{\psi}(\mathbf{p}')\rangle}{\|\mathbf{p}-\mathbf{p}'\|^{n-1}}\,\mathrm{d}^n\mathbf{p}' = \frac{1}{2}\left(p^2-2\mu E\right)|\hat{\psi}(\mathbf{p})\rangle$$

(this is *Equation* (4.6), repeated here for convenience) is equivalent, as desired, to

$$C_n \int_{\mathbb{S}^n} \frac{\Psi(\mathbf{X}')}{\|\mathbf{X}-\mathbf{X}'\|^{n-1}}\,\mathrm{d}\Omega_n' = p_0\Psi(\mathbf{X}).$$

□

The goal we want to achieve now is to show that *Equation* (4.9) is related to the spherical harmonics. As remarked by Bander and Itzykson in [2], we have in $(n+1)$-dimensional space that

$$\frac{1}{\|\mathbf{X}-\mathbf{X}'\|^{n-1}}$$

is the *Green function*[xlv] of the Laplacian operator $\nabla^2_{\mathbb{R}^{n+1}}$. More specifically, we have

$$\nabla^2_{\mathbb{R}^{n+1}} \frac{1}{\|\mathbf{X}-\mathbf{X}'\|^{n-1}} = -(n-1)\Omega_n \delta(\mathbf{X}-\mathbf{X}'),$$

where Ω_n is the area of $\mathbb{S}^n$ given by [1, 4.A.5]

$$\Omega_n = \frac{2\pi^{\frac{n+1}{2}}}{\Gamma\left(\frac{n+1}{2}\right)}. \tag{4.10}$$

Let $\mathbf{X} \in \mathbb{S}^n \setminus \{\mathbf{N}\}$ be fixed, and define the surfaces

$$\begin{cases} \Sigma^1_\varepsilon := \{\mathbf{X}' \in \mathbb{S}^n \setminus \{\mathbf{N}\} \mid (X')^2 = 1 \text{ and } \|\mathbf{X}-\mathbf{X}'\| \geq \varepsilon\}; \\ \Sigma^2_\varepsilon := \{\mathbf{X}' \in \mathbb{S}^n \setminus \{\mathbf{N}\} \mid (X')^2 \leq 1 \text{ and } \|\mathbf{X}-\mathbf{X}'\| = \varepsilon\}, \end{cases}$$

for $\varepsilon \in \mathbb{R}_{>0}$ arbitrary. Lastly, we let Σ_ε be the union of these two surfaces, that is,

$$\Sigma_\varepsilon := \Sigma^1_\varepsilon \cup \Sigma^2_\varepsilon.$$

It is this surface, which can be visualised in *Figure* 4.2 below, that shall be used as the surface of integration in Green's second identity.

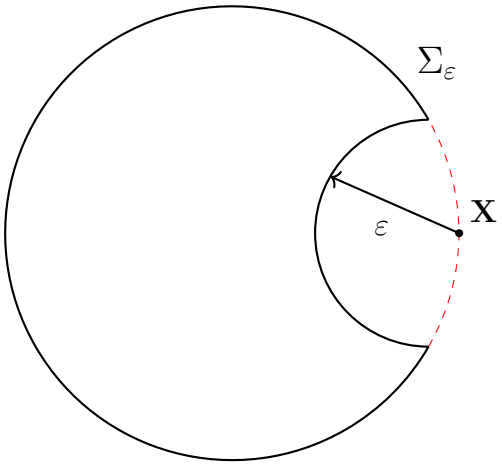

Figure 4.2: The surface Σ_ε is obtained by removing from an n-sphere $\mathbb{S}^n$ a cap of radius ε centred at $\mathbf{X}$, and substituting this by an internal hemisphere with the same radius and centre.

Also let $h \in \mathbb{H}^l_{n+1}$, that is, p is a homogenous harmonic polynomial of degree l in $n+1$ variables.

When we now apply Green's second identity to h and $1/\|\mathbf{X}-\mathbf{X}'\|^{n-1}$, the latter being harmonic everywhere except at $\mathbf{X} = \mathbf{X}'$, then we find[xlvi]

$$0 = \int_{\Sigma_\varepsilon} \left(h(\mathbf{X}') \frac{\partial}{\partial \boldsymbol{\nu}} \frac{1}{\|\mathbf{X}-\mathbf{X}'\|^{n-1}} - \frac{1}{\|\mathbf{X}-\mathbf{X}'\|^{n-1}} \frac{\partial}{\partial \boldsymbol{\nu}} h(\mathbf{X}') \right) \mathrm{d}\Omega'_n.$$

[xlv] See [33, *Chapter* 6].

[xlvi] Note here that the volume inside the surface Σ_ε does not contain $\mathbf{X}$.

Since $\Sigma_\varepsilon = \Sigma_\varepsilon^1 \cup \Sigma_\varepsilon^2$, it is seen that this integral splits into two parts. The first one, taken over Σ_ε^1, tends to an integral over the entire sphere $\mathbb{S}^n$ as $\varepsilon \to 0$. This first integral subsequently has two terms, and for the first term we note that if $X = X' = 1$, then we have

$$\frac{\partial}{\partial \boldsymbol{\nu}} \frac{1}{\|\mathbf{X} - \mathbf{X}'\|^{n-1}} = -\frac{n-1}{2} \frac{1}{\|\mathbf{X} - \mathbf{X}'\|^{n-1}}.$$

The details of this equality we omit, but can be found in [11, *Section* 4.3]. On the other hand, for the second term, we note that $h|_{\mathbb{S}^n} \in \mathscr{Y}_{n+1}^l$, and since $\mathbf{X}' \in \mathbb{S}^n \setminus \{\mathbf{N}\} \subset \mathbb{S}^n$, we have that $h(\mathbf{X}')$ coincides with the spherical harmonics $Y_l^m(\mathbf{X}')$ for all $\mathbf{X}'$, where $m \in \{-l, \dots, -1, 0, 1, \dots, l\}$. Moreover using the properties of homogeneous polynomials, more precisely *Equation* (4.2), we find that

$$\frac{\partial}{\partial \boldsymbol{\nu}} h(\mathbf{X}') = l Y_l^m(\mathbf{X}'),$$

whenever $X' = 1$. Therefore,

$$\begin{aligned} &\int_{\Sigma_\varepsilon^1} \left(h(\mathbf{X}') \frac{\partial}{\partial \boldsymbol{\nu}} \frac{1}{\|\mathbf{X} - \mathbf{X}'\|^{n-1}} - \frac{1}{\|\mathbf{X} - \mathbf{X}'\|^{n-1}} \frac{\partial}{\partial \boldsymbol{\nu}} h(\mathbf{X}') \right) \mathrm{d}\Omega_n' \\ &\qquad \xrightarrow{\varepsilon \to 0} \quad \int_{\mathbb{S}^n} \left(-\frac{n-1}{2} \frac{Y_l^m(\mathbf{X}')}{\|\mathbf{X} - \mathbf{X}'\|^{n-1}} - \frac{l Y_l^m(\mathbf{X}')}{\|\mathbf{X} - \mathbf{X}'\|^{n-1}} \right) \mathrm{d}\Omega_n'. \end{aligned}$$

Next, consider the integral over Σ_ε^2, i.e., over the internal hemisphere with radius ε and centre $\mathbf{X}$. It turns out that

$$\begin{aligned} &\int_{\Sigma_\varepsilon^2} \left(h(\mathbf{X}') \frac{\partial}{\partial \boldsymbol{\nu}} \frac{1}{\|\mathbf{X} - \mathbf{X}'\|^{n-1}} - \frac{1}{\|\mathbf{X} - \mathbf{X}'\|^{n-1}} \frac{\partial}{\partial \boldsymbol{\nu}} h(\mathbf{X}') \right) \mathrm{d}\Omega_n' \\ &\qquad \xrightarrow{\varepsilon \to 0} \quad \frac{n-1}{2} \Omega_n h(\mathbf{X}). \end{aligned}$$

Since $\mathbf{X} \in \mathbb{S}^n \setminus \{\mathbf{N}\} \subset \mathbb{S}^n$, it follows as before that h coincides with the spherical harmonics Y_l^m. Now, combining the previous results, we obtain

$$0 = \frac{n-1}{2} \Omega_n Y_l^m(\mathbf{X}) + \int_{\mathbb{S}^n} \frac{Y_l^m(\mathbf{X}')}{\|\mathbf{X} - \mathbf{X}'\|^{n-1}} \left(-\frac{n-1}{2} - l \right) \mathrm{d}\Omega_n'.$$

Recall that the area of the n-sphere Ω_n is given in *Equation* (4.10). Using this, the above can be rewritten as

$$\begin{aligned} &-\frac{n-1}{2} \frac{2\pi^{\frac{n+1}{2}}}{\Gamma\left(\frac{n+1}{2}\right)} Y_l^m(\mathbf{X}) = \int_{\mathbb{S}^n} \frac{Y_l^m(\mathbf{X}')}{\|\mathbf{X} - \mathbf{X}'\|^{n-1}} \left(-\frac{n-1}{2} - l \right) \mathrm{d}\Omega_n' \\ &\Rightarrow Y_l^m(\mathbf{X}) = \frac{2l + n - 1}{2\pi^{\frac{n+1}{2}}(n-1)} \Gamma\left(\frac{n+1}{2}\right) \int_{\mathbb{S}^n} \frac{Y_l^m(\mathbf{X}')}{\|\mathbf{X} - \mathbf{X}'\|^{n-1}} \mathrm{d}\Omega_n'. \end{aligned}$$

Using the functional relationship of Γ, *Equation* (4.5), we find

$$\Gamma\left(\frac{n+1}{2}\right) = \Gamma\left(\frac{n-1}{2} + 1\right) = \frac{n-1}{2} \Gamma\left(\frac{n-1}{2}\right),$$

and hence

$$Y_l^m(\mathbf{X}) = \frac{2l+n-1}{4\pi^{\frac{n+1}{2}}}\Gamma\left(\frac{n-1}{2}\right)\int_{\mathbb{S}^n}\frac{Y_l^m(\mathbf{X}')}{\|\mathbf{X}-\mathbf{X}'\|^{n-1}}\,\mathrm{d}\Omega_n'. \tag{4.11}$$

Theorem 4.4.3 (Hidden symmetry)**.** The quantum Kepler problem has $SO(n+1)$-symmetry.

Proof. It needs to be shown that *Equation* (4.9) is invariant under rotations in $SO(n+1)$. Let

$$\mathbf{X} \to R\mathbf{X} =: \tilde{\mathbf{X}},$$

be a rotational transformation where $R \in SO(n+1)$. Moreover, define $\tilde{\Psi}(\mathbf{X}) := \Psi(\tilde{\mathbf{X}})$. After applying the transformation, the right-hand side of *Equation* (4.9) becomes $p_0\Psi(\tilde{\mathbf{X}}) = p_0\tilde{\Psi}(\mathbf{X})$. On the other hand, the left-hand side after the transformation is obtained by using the change of variables formula for integrals[(xlvii)],

$$C_n\int_{\mathbb{S}^n}\frac{\Psi(R\mathbf{X}')}{\|R\mathbf{X}-R\mathbf{X}'\|^{n-1}}|J(R\mathbf{X}')|\,\mathrm{d}\Omega_n',$$

where J denotes the Jacobian of the transformation, which is given by $J(R\mathbf{X}') = \det R$. Notice that the integral is still over the n-sphere $\mathbb{S}^n$. Now, recall that

$$SO(n+1) := \{M \in GL\left(\mathbb{R}^{n+1}\right) \mid M^TM = I,\, \det M = 1\},$$

cf. *Definition* 3.1.2. Since $R \in SO(n+1)$, the above allows us to conclude $|J(R\mathbf{X}')| = |\det R| = 1$. Moreover, we find

$$\begin{aligned}\|R\mathbf{X}-R\mathbf{X}'\|^2 &= \|R(\mathbf{X}-\mathbf{X}')\|^2\\ &= \left(R(\mathbf{X}-\mathbf{X}')\right)^T R(\mathbf{X}-\mathbf{X}')\\ &= (\mathbf{X}-\mathbf{X}')^TR^TR(\mathbf{X}-\mathbf{X}')\\ &= (\mathbf{X}-\mathbf{X}')^T(\mathbf{X}-\mathbf{X}')\\ &= \|\mathbf{X}-\mathbf{X}'\|.\end{aligned}$$

Therefore,

$$\|R\mathbf{X}-R\mathbf{X}'\|^{n-1} = \left(\|R\mathbf{X}-R\mathbf{X}'\|^2\right)^{\frac{n-1}{2}} = \|\mathbf{X}-\mathbf{X}'\|^{n-1}.$$

So if we let $\tilde{\Psi}(\mathbf{X}') := \Psi(R\mathbf{X}')$, we have that *Equation* (4.9) after the rotational transformation $X \to \tilde{X}$ becomes

$$C_n\int_{\mathbb{S}^n}\frac{\tilde{\Psi}(\mathbf{X}')}{\|\mathbf{X}-\mathbf{X}'\|^{n-1}}\,\mathrm{d}\Omega_n' = p_0\tilde{\Psi}(\mathbf{X}).$$

When comparing the two, it is seen that only the naming changes and not the equation itself. The conclusion hence follows. □

(xlvii) The change of variables formula can be found in most calculus books, see for example [42].

We can compare the result in *Equation* (4.11) with *Equation* (4.6). It is then seen that

$$\frac{C_n}{p_0} = \frac{2l+n-1}{4\pi^{\frac{n+1}{2}}}\Gamma\left(\frac{n-1}{2}\right).$$

Solving for p_0 gives

$$p_0 = \frac{2\mu k}{\hbar(2l+n-1)}.$$

Recall that $p_0 = \sqrt{-2\mu E}$ and hence the energy levels are

$$\begin{aligned} E &= -\frac{p_0^2}{2\mu} \\ &= -\left(\frac{2\mu k}{\hbar(2l+n-1)}\right)^2 \frac{1}{2\mu} \\ &= -\frac{2\mu k^2}{\hbar^2(2l+n-1)^2}. \end{aligned}$$

Since the spherical harmonics Y_l^m are complete, these are all possible energy levels. Now using the injective and unitary isometry $\mathscr{T}$, cf. *Equation* (4.8), the spectrum of the Hamiltonian $\hat{H}$, $\Lambda_{\hat{H}}$, is given by

$$\Lambda_{\hat{H}} = \left\{ -\frac{2\mu k^2}{\hbar^2(2l+n-1)^2} \mid l \in \mathbb{Z}_{\geq 0} \right\}.$$

The multiplicity of each eigenvalue is equal to $\dim \mathbb{H}^l_{n+1}$, see *Equation* (4.1). This solves the quantum Kepler problem for negative energies.

4.5 Positive Energies ($E > 0$)

In the case of positive energies, we are concerned with unbound states, also called scattering states. The analysis in this case is not trivial given the work for negative energies. This is because for scattering states one finds a *continuous* spectrum $\Lambda_{\hat{H}}$.

Specifically, a complication in the matter is that the *Lemma* 4.4.1 is no longer applicable.

We note that in a di□erent article, Bander and Itzykson extended their work we reviewed in the previous section to scattering states [3]. Here it is concluded that there is no $SO(n+1)$-symmetry, but rather the hidden symmetry is now found in the invariance under the homogeneous Lorentz group $O(d,1)$. Also see [12, *Chapter* 3].

Conclusion

In this thesis, we provided an overview of the symmetries of the Kepler problem. First, a classical stance was taken where we devoted much of our attention towards the conservation of energy, angular momentum, and the Laplace-Runge-Lenz vector. These turned out to be signalling a more fundamental feature: symmetries. It was concluded that the Laplace-Runge-Lenz vector is responsible for unexpected symmetry. Specifically, a symmetry that one can not observe by merely looking at the geometry, but where one has to turn to the dynamics.

By consecutively adopting a quantum mechanical approach, we were able to describe the Kepler problem at a more fundamental level. To essence of us were the commutation relations of the Hamiltonian $\hat{H}$ operator, (orbital) angular momentum operator $\hat{\boldsymbol{\mathcal{L}}}$, and Laplace-Runge-Lenz operator $\hat{\boldsymbol{\mathcal{A}}}$. The latter two both commute with the Hamiltonian operator, therefore establishing an analogue with what one classically calls a conserved quantities. Moreover,

$$\left[\hat{\mathcal{L}}_j, \hat{\mathcal{L}}_k\right] = i\hbar\varepsilon_{jkl}\hat{\mathcal{L}}_l, \qquad \left[\hat{\mathcal{L}}_j, \hat{\mathcal{A}}_k\right] = i\hbar\varepsilon_{jkl}\hat{\mathcal{A}}_l,$$
$$\text{and} \quad \left[\hat{\mathcal{A}}_j, \hat{\mathcal{A}}_k\right] = -2i\hbar\varepsilon_{jkl}\hat{H}\hat{\mathcal{L}}_l.$$

After reviewing the notions of Lie groups and Lie algebras, it was established that exactly the above commutation relations, together with the fact that $\hat{\boldsymbol{\mathcal{L}}}$ and $\hat{\boldsymbol{\mathcal{A}}}$ commute with the Hamiltonian operator, allowed us to conclude Lie algebra $\mathfrak{so}(4)$-symmetry. We commemorate that although we changed our perspective entirely, the Laplace-Runge-Lenz vector promoted to an operator is again relevant in symmetry. This signifies the deep importance of this operator (or, vector, classically).

Finally, following the argument of Bander and Itzykson, we were able to conclude the presence of hidden symmetry of the quantum Kepler problem regardless of the dimension. More specifically, in n dimensions, one has $SO(n+1)$-symmetry. The techniques used in this argument, such as writing the Kepler-Schrödinger equation in the momentum representation and applying a stereographic projection, allowed us to moreover solve the quantum Kepler problem. That is, describing the spectrum of the Hamiltonian operator.

As an outlook, we note that one could devote a lot more research to the symmetries of the Kepler problem. An obvious consideration would be to look at a greater depth at the unbound states where the energy is positive. A topic that is more towards the edge of mathematical progress is the the Ligon-Schaaf regularisation. Here one considers the Ligon-Schaaf mapping which is a modified stereographic projection, allowing for the regularisation of the Kepler problem.

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