Supersymmetry for the Hydrogen Atom

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Abstract

In this thesis it will be shown that the hydrogen atom has a $SU(2) \times SU(2)$ symmetry generated by the quantum mechanical angular momentum and Runge-Lenz vector operators. Additionally, the hydrogenic atom will be studied with supersymmetric methods to identify a supersymmetry that relates different such systems. This thesis is intended to present the material in a manner accessible to people without background in Lie groups and supersymmetry, as well as fill in some calculations between steps that are not spelt out in the literature.
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1 Introduction

In this thesis, we look at symmetry groups that can be generated with constants of motion for the hydrogen atom. First we look at the more well known case of forming a $SU(2)$ using the components of the quantum mechanical angular momentum as generators, as per reference [1], which is the main reference for section 2. After that we will use the Runge-Lenz vector, known to be a conserved quantity for some rotating systems, particularly the $\frac{1}{r^2}$-potential, to form a larger symmetry group. The Runge-Lenz vector is also commonly known as the Laplace-Runge-Lenz vector, though none of the three were first to form it.

This larger group is the $SU(2) \times SU(2)$ Lie group, which can be shown using step operators analogously as for angular momentum. The point of this is that Lie groups are known structures, to which known methods apply. The way we form the $SU(2) \times SU(2)$ makes it look like the group of infinitesimal rotations in four dimensions, though the units are, of course, not the same.

Both of these symmetries correspond to the degeneracy of the energy levels of the hydrogen atom. They are related via the conserved quantities. This is not new knowledge; for example, was discussed by Pauli already back in 1926 ([8]).

Furthermore, we will use the notion of supersymmetry to look at some additional symmetry of hydrogenic atoms. For this, we will require some more general information on how to apply supersymmetry to quantum mechanical systems. The specific approach we will take to applying supersymmetry in section 3 comes from reference [3], but the basic framework existed earlier, see e.g. reference [9]. It has since been referred to in a number of other works, such as reference [5]. Further reading can also be done in reference [6].

Supersymmetry originally comes from theoretical high-energy physics. There, $Q$ is an operator that operates on a boson, producing a fermion. This gives an extra particle for each particle in the standard model and gives us the "minimal supersymmetric standard model". This model does not contain any other additional heavier particles. As compared to the standard model, the supersymmetric version alleviates the so-called hierarchy problem. More on this can be found e.g. in reference [4].

The purpose of considering these different types of symmetry together is that we are able to draw parallels between their structure and properties.

None of the considerations in this thesis are truly new. The thesis contains no material that cannot be found elsewhere, but gathers the relevant information in one place and presents some calculations that have been skipped in the original
literature. Compare for example reference [7], which discusses much the same ma-
terial, as well as other things, without going through the $SU(2) \times SU(2)$ symmetry 
extensively.

In the entire thesis, our model for hydrogenic atoms will be the most idealized 
version. As such we will always have one electron and neglect such things as 
corrections for spin, relativistic effects or finite size of the nucleus.

Some background on the generators of $SU(2) \times SU(2)$ can be found in Appendix 
A.
2 The Hydrogen Atom

Known conserved quantities of the hydrogen atom include the angular momentum \( L \) and the Runge-Lenz vector \( \mathbf{A} \). As such, both commute with the Hamiltonian \( \mathbf{H} \). We will not prove this, but it can be found elsewhere, as in reference [1], section 9.

We will generally be working with these conserved quantities as quantum mechanical operators, which are used on state vectors. The state vectors are usually described using wave functions in position or momentum space. In position space \( \mathbf{x} \) is a multiplicative operator and \( \mathbf{p} \) is a differential operator. In momentum space it is the other way around. Two quantum mechanical operators do not necessarily commute, but as long as two operators are constructed from \( \mathbf{x} \) and \( \mathbf{p} \) their commutator can be determined from the canonical commutation relations for \( \mathbf{x} \) and \( \mathbf{p} \).

In the following subsections it will be shown that the angular momentum operators generates a \( SU(2) \) and that the angular momentum operators and the Runge-Lenz vector operators together generate a \( SU(2) \times SU(2) \).

2.1 Angular Momentum

We wish to show that \( \mathbf{L} \) forms a group with generators, such that

\[
[L_i, L_j] = \sum_{k=1}^{3} i\hbar \epsilon_{ijk} L_k .
\] (2.1)

In quantum mechanics, we define angular momentum as

\[
\mathbf{L} = \frac{1}{2} (\mathbf{x} \times \mathbf{p} - \mathbf{p} \times \mathbf{x})
\] (2.2)

where \( \mathbf{x} \) and \( \mathbf{p} \) are the operators for position and momentum, respectively. We need to define \( \mathbf{L} \) in this way rather than the way we do classically, because \( \mathbf{x} \) and \( \mathbf{p} \) do not commute.

The angular momentum is a conserved quantity, and accordingly satisfies \([\mathbf{L}, H] = 0\). \( H \) for this system is taken as

\[
H = \frac{p^2}{2m} - \frac{k}{r}.
\] (2.3)

As per the rules for the cross product, we have

\[
L_1 = x_2 p_3 - x_3 p_2
\] (2.4)
\[ L_2 = x_3 p_1 - x_1 p_3 \]  
(2.5)

\[ L_3 = x_1 p_2 - x_2 p_1 . \]  
(2.6)

These are the same formulas as in the classical case, except that we are working with operators. From now on, we will only give the calculation of a single sample equation for a component, followed by the more general summation formula when relevant.

We need to check the commutators for the components of \( L \), but first we determine those for \( L_i \) with \( x_i \) and \( p_i \). Recall that the canonical commutation relations are

\[ [x_i, p_j] = i\hbar \delta_{ij} \]  
(2.7)

and

\[ [x_i, x_j] = [p_i, p_j] = 0 \]  
(2.8)

for \( i, j = 1, 2, 3 \).

The following commutators are easy, as \( L_i \) does not contain \( x_i \) or \( p_i \).

\[ [L_i, x_i] = [L_i, p_i] = 0 . \]  
(2.9)

The other commutators we need to actually calculate. We will be using the relations

(2.10)

and

(2.11)

Using equations (2.7), (2.8), (2.10) and (2.11), we find that
\[ [L_1, x_2] = [x_2 p_3 - x_3 p_2, x_2] \]
\[ = [x_2 p_3, x_2] - [x_3 p_2, x_2] \]
\[ = x_2 [p_3, x_2] + [x_2, x_2] p_3 - x_3 [p_2, x_2] - [x_3, x_2] p_2 \] 
\[ = 0 + 0 + i \hbar x_3 - 0 \]
\[ = i \hbar x_3 . \]  

(2.12)

Calculating all the commutators of \( L_1, L_2 \) and \( L_3 \) with all the components of \( x \) and \( p \) analogously, we can see that we have

\[ [L_i, x_j] = \sum_{k=1}^{3} i \hbar \epsilon_{ijk} x_k \]  

(2.13)

and

\[ [L_i, p_j] = \sum_{k=1}^{3} i \hbar \epsilon_{ijk} p_k . \]  

(2.14)

Having these commutators, we can continue to calculate \([L_i, L_j]\). Trivially, we have

\[ [L_i, L_i] = 0 . \]  

(2.15)

For the commutators of different components, we get

\[ [L_1, L_2] = [L_1, x_3 p_1 - x_1 p_3] \]
\[ = [L_1, x_3 p_1] - [L_1, x_1 p_3] \]
\[ = x_3 [L_1, p_1] + [L_1, x_3] p_1 - x_1 [L_1, p_3] - [L_1, x_1] p_3 \]
\[ = 0 - i \hbar x_2 p_1 + i \hbar x_1 p_2 - 0 \]
\[ = i \hbar (x_1 p_2 - x_2 p_1) \]
\[ = i \hbar L_3 . \]  

(2.16)

Similarity, we find that

\[ [L_3, L_1] = i \hbar L_2 \]  

(2.17)

and
\[ [L_2, L_3] = i\hbar L_1. \]  

Equations (2.16)-(2.18) together with (2.15) give us (2.1). This is what we needed for the components of \( \mathbf{L} \) to be the generators of \( SU(2) \). As such, we can also define the step operators \( L_\pm \):

\[ L_\pm = L_1 \pm iL_2. \]  

The step operators satisfy the commutation relations

\[ [L_+, L_-] = 2\hbar L_3 \]  

and

\[ [L_3, L_\pm] = \pm \hbar L_\pm. \]

### 2.2 Runge-Lenz Vector

The Runge-Lenz Vector is another quantity that is conserved for the system we are considering. Classically it is given by

\[ \mathbf{A} = \mathbf{p} \times \mathbf{L} - mk \frac{\mathbf{x}}{r} \]  

where \( r = |\mathbf{x}| \), \( m \) is the mass of the electron and \( k \) is the constant in the electrical force \( \mathbf{F} \) as per

\[ \mathbf{F} = -\frac{k \mathbf{x}}{r^3}. \]

In quantum mechanics, the Runge-Lenz vector is defined as

\[ \mathbf{A} = \frac{1}{2}(\mathbf{p} \times \mathbf{L} - \mathbf{L} \times \mathbf{p}) - mk \frac{\mathbf{x}}{r} \]  

where \( \mathbf{p}, \mathbf{L}, \mathbf{x}, r \) are now quantum mechanical operators. This means that the Runge-Lenz vector does not have the same form in quantum mechanics as it has classically. The reason for this is that the components of \( \mathbf{p} \) and \( \mathbf{L} \) do not commute for different indices of the vectors, in the same manner as \( \mathbf{x} \) and \( \mathbf{p} \). \( \mathbf{A} \) is a conserved quantity, that is \( [\mathbf{A}, H] = 0 \). Explicitly, we get \( \mathbf{A} \) in components as
\[ A_1 = \frac{1}{2} (p_2 L_3 - p_3 L_2 - (L_2 p_3 - L_3 p_2)) - mk \frac{x_1}{r} \]
\[ = \frac{1}{2} (p_2 L_3 - p_3 L_2 - L_2 p_3 + L_3 p_2) - mk \frac{x_1}{r} \]
\[ = \frac{1}{2} (p_2 L_3 - p_3 L_2 - (p_3 L_2 - i \hbar p_1) + (p_2 L_3 + i \hbar p_1)) - mk \frac{x_1}{r} \]
\[ = \frac{1}{2} (p_2 L_3 - p_3 L_2 - p_3 L_2 + i \hbar p_1 + p_2 L_3 + i \hbar p_1) - mk \frac{x_1}{r} \]
\[ = p_2 L_3 - p_3 L_2 + i \hbar p_1 - mk \frac{x_1}{r} \] (2.25)

and analogously for \( A_2 \) and \( A_3 \). Note that we have used equation (2.14). We can summarize the components of \( A \) as

\[ A_i = \left( \sum_{j,k=1}^{3} \epsilon_{ijk} p_j L_k \right) + i \hbar p_i - mk \frac{x_i}{r}. \] (2.26)

We need to calculate \([A_i, A_j]\) and \([L_i, A_j]\). However, to do so we need to find a number of other commutators first. We need the following relations, which are equations (2.2.23) in reference [2].

\[ [p_i, F(x)] = -i \hbar \frac{\partial F(x)}{\partial x_i}, \] (2.27)

\[ [x_i, F(x)] = 0. \] (2.28)

Equations (2.27) and (2.28) are valid for functions \( F(x) \) with convergent Taylor series about zero. For example, we can easily check that it holds for

\[ F(x) = x \] (2.29)

and

\[ F(x) = x^2. \] (2.30)

This gives us
\[
[p_1, x_1 \frac{1}{r}] = -ih \frac{\partial}{\partial x_1} \left( \frac{x_1}{\sqrt{x_1^2 + x_2^2 + x_3^2}} \right) \\
= -ih \frac{x_2^2 + x_3^2}{(x_1^2 + x_2^2 + x_3^2)^{3/2}} \\
= -ih \frac{x_2^2 + x_3^2}{r^3} ,
\]

while

\[
[p_1, x_2 \frac{1}{r}] = -ih \frac{\partial}{\partial x_1} \left( \frac{x_2}{\sqrt{x_1^2 + x_2^2 + x_3^2}} \right) \\
= ih \frac{x_1 x_2}{(x_1^2 + x_2^2 + x_3^2)^{3/2}} \\
= ih \frac{x_1 x_2}{r^3} .
\]

By the same methods, we can determine all 9 commutators of the type \([p_i, \frac{x_j}{r}]\). The others are omitted to save space.

Using the earlier commutators, we can find

\[
[L_1, x_1 \frac{1}{r}] = [x_2 p_3 - x_3 p_2, x_1 \frac{1}{r}] \\
= [x_2 p_3, x_1 \frac{1}{r}] - [x_3 p_2, x_1 \frac{1}{r}] \\
= x_2[p_3, x_1 \frac{1}{r}] + [x_2, x_1 \frac{1}{r}] p_3 - x_3[p_2, x_1 \frac{1}{r}] - [x_3, x_1 \frac{1}{r}] p_2 \\
= x_2 i h \frac{x_1 x_3}{r^3} + 0 - x_3 i h \frac{x_1 x_2}{r^3} - 0 \\
= 0 .
\]

In the same manner, we get all the other commutators. The results can be summarized as

\[
[L_i, x_j \frac{1}{r}] = \sum_{k=1}^{3} i \hbar \epsilon_{ijk} \frac{x_k}{r} 
\]
for \(i, j = 1, 2, 3\). At this point, we can handle \([L_i, A_j]\). We get
\[ [L_1, A_1] = [L_1, p_2 L_3 - p_3 L_2 + i\hbar p_1 - mk \frac{x_1}{r}] = [L_1, p_2 L_3] - [L_1, p_3 L_2] + i\hbar L_1, p_1] - mk [L_1, \frac{x_1}{r}] = p_2 [L_1, L_3] + [L_1, p_2] L_3 - p_3 [L_1, L_2] - [L_1, p_3] L_2 + 0 - 0 \]
\[ = -i\hbar p_2 L_2 + i\hbar p_3 L_3 - i\hbar p_3 L_3 + i\hbar p_2 L_2 = 0. \]

By analogous calculations, we get
\[ [L_i, A_j] = \sum_{k=1}^{3} i\hbar \epsilon_{ijk} A_k \]
for \( i, j = 1, 2, 3. \)

Finally, we also calculate \([A_i, A_j]\). Trivially,
\[ [A_i, A_i] = 0. \]

For the other commutators, we will need \([p_i, A_j]\) and \([A_i, \frac{x_i}{r}]\). We have
\[ [p_1, A_1] = [p_1, p_2 L_3] - [p_1, p_3 L_2] + i\hbar [p_1, p_1] - mk [p_1, \frac{x_1}{r}] = p_2 [p_1, L_3] + [p_1, p_2] L_3 - p_3 [p_1, L_2] - [p_1, p_3] L_2 + 0 - mk [p_1, \frac{x_1}{r}] = -i\hbar p_2 p_2 + 0 - i\hbar p_3 p_3 + 0 - mk [p_1, \frac{x_1}{r}] = -i\hbar (p_2^2 + p_3^2) - mk [p_1, \frac{x_1}{r}] \]
and
\[ [A_1, \frac{x_2}{r}] = [p_2 L_3 - p_3 L_2 + i\hbar p_1 - mk \frac{x_1}{r}, \frac{x_2}{r}] = p_2 [L_3, \frac{x_2}{r}] + [p_2, \frac{x_2}{r}] L_3 - p_3 [L_2, \frac{x_2}{r}] - [p_3, \frac{x_2}{r}] L_2 + i\hbar [p_1, \frac{x_2}{r}] - mk [\frac{x_1}{r}, \frac{x_2}{r}] = -i\hbar p_2 \frac{x_1}{r} + i\hbar \frac{x_2}{r} - p_3 L_3 - 0 - i\hbar \frac{x_2 x_3}{r^3} L_2 + i^2 \hbar^2 \frac{x_1 x_2}{r^3} + 0. \]

Analogous calculations for the remaining components are omitted to save space.

Now we have all the commutators we need to calculate \([A_i, A_j]\). As the cal-
calculation is a bit long, it is given in Appendix B as equations (6.1)-(6.6). The calculations for the other two commutator follow analogously. To give all three commutators at once, we can write

\[ [A_i, A_j] = -2i\hbar m \sum_{k=1}^{3} H\epsilon_{ijk}L_k \, . \] (2.40)

We see that we need to define a normalized \( K \) to get the proper commutators for a \( SU(2) \times SU(2) \). We can define it as

\[ K = \frac{A}{\sqrt{-2mH}} \] (2.41)

In order for this expression to make sense, we must consider \( H \) to be replaced by an eigenvalue. This implies in particular that we must restrict ourselves to working with the bound states, as these are the ones with negative energies. We may then treat \( H \) as a constant, as it commutes with all other operators involved. We then get

\[ [L_i, K_j] = \sum_{k=1}^{3} i\hbar\epsilon_{ijk}K_k \, . \] (2.42)

as well as

\[ [K_i, K_j] = \sum_{k=1}^{3} i\hbar\epsilon_{ijk}L_k \, . \] (2.43)

To reformulate this as the commutation relations of a \( SU(2) \times SU(2) \), we define the ladder operators \( L^\pm \) as

\[ L^\pm = \frac{1}{2}(L \pm K) \] (2.44)

Clearly, these are also conserved quantities. By direct calculation from equations (2.1), (2.41), (2.42) and (2.43), we have the following commutators:

\[ [L^+_i, L^+_i] = \sum_{k=1}^{3} i\hbar\epsilon_{ijk}L^+_k \, , \] (2.45)

\[ [L^-_i, L^-_i] = \sum_{k=1}^{3} i\hbar\epsilon_{ijk}L^-_k \, , \] (2.46)

\[ [L^+_i, L^-_i] = 0 \, . \] (2.47)

Thus, we do indeed have two separate \( SU(2) \) symmetries.
3 Supersymmetry

3.1 Supersymmetric Framework

There is also another symmetry that can be identified in hydrogenic atoms. It is called a supersymmetry, and will be discussed in this section. Following reference [3] p. 929-930, we consider two one-dimensional systems with potentials

$$V_± = \frac{(U')^2}{8} \mp \frac{U''}{4}$$  \hspace{1cm} (3.1)

with $U = U(x)$ as some given function that characterizes the systems.

We summarize the two Hamiltonians for these systems by a single Hamiltonian with a $2 \times 2$-matrix structure, according to

$$H = \begin{pmatrix} H_- & 0 \\ 0 & H_+ \end{pmatrix} = \frac{p^2}{2m} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} V_- & 0 \\ 0 & V_+ \end{pmatrix}.$$  \hspace{1cm} (3.2)

The crucial observation is now that this combined Hamiltonian can be rewritten in terms of operators $Q$ and $\overline{Q}$, defined as

$$Q = (p - i \frac{U'}{2})\sigma_+$$  \hspace{1cm} (3.3)\]

and

$$\overline{Q} = (p + i \frac{U'}{2})\sigma_-$$  \hspace{1cm} (3.4)

where

$$\sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$$  \hspace{1cm} (3.5)

and

$$\sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}.$$  \hspace{1cm} (3.6)

With these operators, we have

$$\begin{pmatrix} 0 & 0 \\ 0 & H_+ \end{pmatrix} = \frac{1}{2} \overline{Q}Q$$  \hspace{1cm} (3.7)

and

$$\begin{pmatrix} H_- & 0 \\ 0 & 0 \end{pmatrix} = \frac{1}{2} Q\overline{Q}.$$  \hspace{1cm} (3.8)

It follows in particular that the Hamiltonian can be expressed as
\[ H = \frac{1}{2}(Q\overline{Q} + \overline{Q}Q) . \]  

(3.9)

As a shorthand for equations (3.7) and (3.8), we will use

\[ H_+ = \frac{1}{2}Q\overline{Q} \]  

(3.10)

and

\[ H_- = \frac{1}{2}\overline{Q}Q . \]  

(3.11)

The spectra of \( H_+ \) and \( H_- \) are related to each other by the operator \( Q \). We can see this in the following manner: Assuming \( \psi_n \) to be an eigenstate of \( H_+ \), with

\[ H_+\psi_n = E_n\psi_n , \]  

(3.12)

we get

\[ H_- (Q\psi_n) = \frac{1}{2}Q\overline{Q}(Q\psi_n) = Q\left(\frac{1}{2}Q\overline{Q}\psi_n\right) = Q(E_n\psi_n) = E_n(Q\psi_n) . \]  

(3.13)

This means that \( H_+ \) and \( H_- \) have the same eigenvalues, except that the lowest energy state will be missing for \( H_- \). Indeed, it is easily verified that

\[ \psi_0 = e^{-\frac{1}{2}U(x)} . \]  

(3.14)

satisfies

\[ Q\psi_0 = 0 . \]  

(3.15)

Together with equations (3.10) and (3.11) we get that \( \psi_0 \) is an eigenstate of \( H_+ \) with eigenvalue 0. However, \( Q\psi_0 = 0 \) is not a non-trivial eigenstate of \( H_- \). On the other hand, provided that the function \( U \) behaves sufficiently well for \( x \to \pm\infty \), the state \( Q\psi_n \) is normalizable and is thus a valid non-trivial eigenstate of \( H_- \). Thus, \( H_+ \) has one eigenvalue that is not an eigenvalue for \( H_- \), while all the others are the same.

Conceptually the so obtained supersymmetry is rather different than the Lie group symmetries in section 2, but there are some computational parallels. For example, the operators \( \sigma_\pm \) in equations (3.5) and (3.6) are similar to the step operators \( L_\pm \) from equation (2.19).
3.2 Hydrogen Atom

We will now analyse the spectrum of hydrogenic atoms with the help of this framework. We will be following reference [3], p. 932-934. We consider the radial part of the Schrödinger equation, i.e.

\[
\left( -\frac{1}{2} \frac{d^2}{dy^2} - \frac{1}{y} + \frac{l(l+1)}{2y^2} \right) \chi_{nl}(y) = E_n \chi_{nl}(y)
\]  

(3.16)
as per reference [3], equation (29). Here, \( \frac{1}{y} \) is the Coulomb attraction and \( \frac{l(l+1)}{2y^2} \) is the angular momentum barrier. Also, we are using the abbreviation

\[
y = Z \frac{mc^2}{\hbar^2} r.
\]  

(3.17)

\( Z \) is the atomic number of the hydrogenic atom. This \( y \) is a dimensionless quantity, which causes the eigenvalues we will obtain to become dimensionless as well. Despite this, we will refer to such eigenvalues as those they otherwise correspond to, such as in equation (3.18) below.

The energy eigenvalues are

\[
E_n = \frac{1}{2n^2}.
\]  

(3.18)

It turns out that we can express the Hamiltonian of this system in the supersymmetric form from equation (3.1): the corresponding function \( U(y) \) is

\[
U(y) = \frac{2y}{l+1} - 2(l+1) \ln(y),
\]  

(3.19)

which we can see by using \( U \) to reproduce the potential as \( V_+ \) (as given in equation (3.2)) up to an irrelevant additive constant. Indeed, using equation (3.1), we get

\[
V_+(y) = \frac{(U')^2}{8} - \frac{U''}{4}
\]  

\[
= \frac{1}{2} \left( \frac{1}{(l+1)^2} - \frac{2}{y} + \frac{(l+1)^2}{y^2} - \frac{(l+1)}{y^2} \right)
\]  

\[
= \frac{1}{2} \frac{1}{(l+1)^2} - \frac{1}{y} + \frac{1}{2} \frac{l^2 + l}{y^2}
\]  

\[
= \frac{1}{2} \frac{1}{(l+1)^2} - \frac{1}{y} + \frac{1}{2} \frac{l(l+1)}{y^2}.
\]  

(3.20)

Having \( U \), we also calculate
\[ V_-(y) = \frac{(U')^2}{8} + \frac{U''}{4} \]
\[= \frac{1}{2} \left( \frac{1}{(l+1)^2} - \frac{2}{y} + \frac{(l+1)^2}{y^2} \right) + \frac{1}{2} \left( \frac{1}{(l+1)^2} - \frac{2}{y} + \frac{l^2 + 2l + 1 + l + 1}{y^2} \right) \]
\[= \frac{1}{2} \frac{1}{(l+1)^2} - \frac{1}{y} + \frac{1}{2} \frac{l^2 + 3l + 2}{y^2} \]
\[= \frac{1}{2} \frac{1}{(l+1)^2} - \frac{1}{y} + \frac{1}{2} \frac{(l+1)(l+2)}{y^2}. \]

It is now crucial to note that \( V_- \) is of the same form as \( V_+ \), and differs from it only by the replacement
\[ l \mapsto l + 1. \quad (3.22) \]

We can also calculate \( Q \) and \( \overline{Q} \). As per equations (3.3) and (3.4), they become
\[ Q = \left( p - \frac{1}{l+1} + \frac{(l+1)}{y} \right) \sigma_+ \quad (3.23) \]
and
\[ \overline{Q} = \left( p + \frac{1}{l+1} - \frac{(l+1)}{y} \right) \sigma_- . \quad (3.24) \]

Finding the eigenvalues of the corresponding Hamiltonians is a little involved, but can be achieved by using the variable \( x = \ln(y) \) for \( H_+ \), which gives us a so-called Morse potential. Shifting the lowest energy eigenvalue to zero, we get a new potential
\[ \overline{V}_+(x) = \frac{1}{2n^2} e^{2x} - e^x + \frac{1}{2} \left( \frac{1}{2} - n \right). \quad (3.25) \]

The Hamiltonian \( H_+ \) has, as per reference [3], the eigenvalues
\[ E_{n,l} = \frac{1}{2} (n + l)(n - l - 1), \quad (3.26) \]
with \( 0 \leq l \leq n - 1 \). For this potential, we have
\[ \overline{U}(x) = \frac{2}{n} e^x + 2 \left( \frac{1}{2} - n \right) x. \quad (3.27) \]

Using this, we find that
\( \tilde{V}_-(x) = \frac{1}{2n^2} e^{2x} - \left(1 - \frac{1}{n}\right) e^x + \frac{1}{2} \left(\frac{1}{2} - n\right) . \)  

(3.28)

According to the discussion in section 3.1, \( \tilde{V}_- \) has the same eigenvalues as \( \tilde{V}_+ \), except that it is lacking the eigenvalue zero. This is the eigenvalue for which \( l = n - 1 \).

Reformulating this in terms of the variable \( y \), equation (3.16) becomes

\[ \tilde{H}_+(y) \chi_{nl}(y) = E_n \chi_{nl}(y) \]  

(3.29)

At this point, it is a good idea to check that inserting equation (3.19) into equation (3.14) does give us the state we expect.

\[ \psi_0 = e^{-\frac{1}{2} \left(\frac{2}{n+1} - 2(l+1) \ln(y)\right)} e^{-\frac{1}{n+1} e^{(l+1) \ln(y)}} = y^{l+1} e^{-\frac{1}{n+1}} \]  

(3.30)

Inserting \( l = 0 \), which is correct for \( n = 1 \), and equation (3.17), we get

\[ \psi_0 = Z \frac{me^2}{\hbar^2} r e^{-\left(-\frac{me^2}{\hbar^2} r\right)} . \]  

(3.31)

Apart from the constant, which is a matter of normalization, this is the state we were expecting.

Continuing, we get

\[ \tilde{H}_-(y) \chi_{nl}(y) = \left(-\frac{1}{2} \frac{d^2}{dy^2} - \left(1 - \frac{1}{n}\right) \frac{1}{y} + \frac{1}{2} \frac{l(l+1)}{y^2}\right) \chi_{nl}(y) \]  

(3.32)

By dividing the entire equation by \( (1 - \frac{1}{n})^2 \) and defining

\[ z = (1 - \frac{1}{n}) y \]  

(3.33)

we get

\[ \tilde{H}_- \chi_{nl}(z) = \left(-\frac{1}{2} \frac{d^2}{dz^2} - \frac{1}{z} + \frac{1}{2} \frac{l(l+1)}{z^2}\right) \chi_{nl}(z) \]  

(3.34)
Since $y$ contains $Z$, we can view the change $y \mapsto z$ as taking $Z \mapsto Z(1 - 1/n)$. Now the only difference between equations (3.32) and (3.34) is that the first applies to $n$ while the second applies to $n - 1$. As such, our supersymmetric operator $Q$ implements the simultaneous change of

$$n \mapsto n - 1$$

and

$$Z \mapsto Z(1 - 1/n).$$

(3.35)

(3.36)

Three examples of this transition, with the zero eigenvalue missing for $H_-$ are shown in figure 1. The figure makes it clear that these supersymmetrical transitions indeed relate hydrogenic atoms of different charge.

![Figure 1: Supersymmetric spectrum of simultaneous transition $n \mapsto n - 1$ and $Z \mapsto Z(1 - 1/n)$ for a) $n = Z = 2$ b) $n = Z = 3$ c) $n = Z = 4$](image)

The usefulness of the supersymmetrical operators $Q$ and $\overline{Q}$ we have constructed may be a bit difficult to evaluate. We can interpret the result as having found a symmetry between states for hydrogenic ions of different atomic number $Z$, such that we have equal energy eigenvalue for $n$ and $Z$ and for $n - 1$ and $Z(1 - 1/n)$, with both ions having the same $l$.

This symmetry is present in this simple model of a hydrogenic atom. However, when comparing this theoretic prediction with measurements, one must be aware of the fact that a more accurate treatment of a system like this should involve other terms, such as relativistic perturbations. In addition to this, the transition represented by $Q$ cannot usually take place, as it involves a simultaneous change of state of the electron and the charge of the nucleus. Still, it is interesting that we can find this additional symmetry for the model of the hydrogenic atom.
4 Conclusions

In this thesis, we were to look over the standard symmetries for the hydrogen atom and some further supersymmetry that can be applied when studying the most simple model of a hydrogenic atom. To do so, we had to go through several different steps.

We have calculated the commutators for $L$ and $A$ for the hydrogen atom, seeing that we can use them to form the generators of a $SU(2) \times SU(2)$ symmetry.

To do so, we had to introduce the operator $K$ of equation (2.41) and determine the commutators $[L_i, L_j]$, $[L_i, K_j]$ and $[K_i, K_j]$ for $i, j = 1, 2, 3$. We did this in smaller steps, forming other commutators, which we then used to keep the calculations relatively brief.

We have also applied supersymmetry to the hydrogenic atom, finding a similar symmetry for simultaneous transitions of $n \to n - 1$ and $Z \to Z(1 - 1/n)$. This required us to first review the supersymmetric framework. This involved using Hamiltonians $H_{\pm}$ with potentials $V_{\pm}$ formed from the derivatives of a characteristic function $U$ of the system. We then applied this to the simplest model of a hydrogenic atom, finding $V_{\pm}, Q_{\pm}$ and $H_{\pm}$.

The resulting supersymmetric relations were interpreted as a symmetry between different hydrogenic ions.

Both of the symmetries we have considered are broken if we apply corrections to the Hamiltonians involved, but the results are still important as long as the corrections are sufficiently small.

It is worth noting that the standard quantum mechanical symmetry from section 2 shares some properties with the supersymmetry from section 3. For example, they both involve step operators. We conclude that they both are symmetries that apply to the hydrogenic atom, even if they are of rather different types.
5 Appendix A

This section is devoted to showing how the group SO(3) is defined with the skew-symmetric epsilon tensor, as well as its commutation relations.

The skew-symmetric epsilon tensor $\epsilon_{ijk}$ is defined as taking the value of 1 for even permutations of $i, j, k$ and $-1$ for odd permutations. It is otherwise equal to zero. This makes it useful for some summation formulas, such as the cross product. For the cross-product $C = A \times B$, the components $C_i$ can be expressed through the components of $A$ and $B$ as

$$C_i = \sum_{j,k=1}^{3} \epsilon_{ijk} A_j B_k .$$  \hspace{1cm} (5.1)

5.1 Symmetry Groups

Describing a group using generators is often useful. In our case, the actual Lie groups have an infinite number of elements, but have a small, finite, number of generators. The generators form a Lie algebra.

Often, we can describe an element $E$ of a Lie group with generators $A_1$ through $A_n$ as

$$E = \exp(i \sum_{k=1}^{n} b_k A_k ) .$$  \hspace{1cm} (5.2)

We will only be using the group $SU(2)$ and the $SU(2) \times SU(2)$ in this thesis, and for these two groups equation (5.2) holds.

As per reference [1] $SU(2)$ is a Lie group with generators $A_1$, $A_2$ and $A_3$ such that

$$[A_i, A_j] = \sum_{j,k=1}^{3} \epsilon_{ijk} A_k .$$  \hspace{1cm} (5.3)

In quantum mechanics, it is conventional to rescale the operators such that there is also a factor of $ih$. The $SU(2) \times SU(2)$ is similar, consisting of two different $SU(2)$. It has three more generators $B_1$, $B_2$ and $B_3$, such that

$$[B_i, B_j] = \sum_{j,k=1}^{3} \epsilon_{ijk} A_k ,$$  \hspace{1cm} (5.4)

$$[A_i, B_j] = \sum_{j,k=1}^{3} \epsilon_{ijk} B_k .$$  \hspace{1cm} (5.5)
These are not manifestly the commutators for two different $SU(2)$ symmetries, but instead for the group $SO(4)$ of rotations in four dimensions, that has 6 generators. This $SO(4)$ is however the same as $SU(2) \times SU(2)$, which can be made explicit by reformulating equations (5.3)-(5.5) by forming step operators. This is done as per equation (2.44).
6 Appendix B

Equations (6.1)-(6.6) has been moved to this appendix to save space in section 2.2. In the calculation, most of the results for commutators from section 2 are used, as well as the rules for working with commutators. Here, only the calculation of $[A_1, A_2]$ is given, but the commutators with other components of the Runge-Lenz vector can be calculated analogously.

First, we use the definition of $A_1$ and the rules for addition and multiplication with constant in a commutator.

$$
[A_1, A_2] = \left[ p_2 L_3 - p_3 L_2 + i\hbar p_1 - mk x_1, A_2 \right] \\
= p_2 [L_3, A_2] + [p_2, A_2] L_3 - p_3 [L_2, A_2] - [p_3, A_2] L_2 (6.1) \\
+ i\hbar [p_1, A_2] + mk \left[ A_2, \frac{p_1}{r} \right].
$$

Then, we insert previously known commutators from section (2).

$$
[A_1, A_2] = -i\hbar p_2 A_1 + \left( -i\hbar(p^2_1 + p^2_3) + mk i\hbar \frac{x_1^2 + x_2^2}{r^2} \right) L_3 \\
- \left( i\hbar p_2 p_3 - mk i\hbar \frac{x_1 x_2}{r^2} \right) L_2 + i\hbar \left( i\hbar p_1 p_2 - mk i\hbar \frac{x_1 x_2}{r^2} \right) (6.2) \\
+ mk i\hbar \left( \frac{x_1 x_3}{r^2} L_1 + \frac{x_2 x_3}{r^2} L_3 - p_1 \frac{z_3}{r} + i\hbar \frac{x_1 x_2}{r^2} \right).
$$

Now, we try to put multiplicative constants outside the expressions containing operators, and group similar expressions together.

$$
[A_1, A_2] = i\hbar(-p_2 A_1 - (p^2_1 + p^2_3)L_3 - p_2 p_3 L_2 \\
+ \left( \frac{x_1^2 + x_2^2}{r^2} L_3 + \frac{x_1 x_3}{r^2} L_2 + \frac{x_2 x_3}{r^2} L_1 + \frac{x_3^2 + x_2^2}{r^2} L_3 - p_1 \frac{z_3}{r} \right) (6.3) \\
+ i\hbar \left( p_1 p_2 + mk \left( -\frac{x_1 x_3}{r^2} + \frac{x_2 x_2}{r^2} \right) \right)).
$$

At this point, we insert the definition of $A_1$, and continue simplifying the expression.

$$
[A_1, A_2] = i\hbar(-p_2 \left( p_3 L_3 - p_3 L_2 + p_1 L_2 + i\hbar p_1 - mk x_1 \right) - (p^2_1 + p^2_3) L_3 \\
+ mk \left( \frac{x_1^2 + x_2^2 + 2x_3^2}{r^2} L_3 - \frac{x_2^2}{r^2} - p_1 \frac{z_3}{r} \right) \right). (6.4)
$$

At this point, several terms cancel each other out. We keep simplifying.

$$
[A_1, A_2] = i\hbar \left( -p_2^2 L_3 - i\hbar p_1 p_2 + mk \left( p_2 \frac{x_1}{r} - p_1 \frac{x_2}{r} + \frac{r^2}{r^2} L_3 \right) + \frac{i\hbar p_1 p_2}{r} \right) (6.5) \\
= i\hbar \left( -p^2 L_3 + mk \frac{1}{r} L_3 + mk(p_2 x_1 - p_1 x_2) \frac{1}{r} \right).
$$

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Finally, we identify $L_3$ and finish simplifying the expression.

\[
[A_1, A_2] = i\hbar (-p^2 L_3 + mk_1^2 L_3 + mk_2^2 L_3) \\
= -2i\hbar m \left( \frac{p^2}{2m} - \frac{k}{r} \right) L_3.
\] (6.6)

References

[1] G. ’t Hooft, B.Q.P.J. de Wit and M.J.G. Veltman, Lie Groups In Physics, Utrecht University, 25/06/07


