The Dirac Equation for a Particle in a Spherical Box Potential with Application in Bag Modeling

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Abstract

The Dirac equation is a relativistic wave equation and was the first equation to capture spin in relativistic quantum mechanics. Here, the Dirac equation will be derived and solved for a particle in a spherical box potential. Comparisons to the non-relativistic Schrödinger equation as well as to a relativistically corrected Schrödinger equation will be made. Applications of the Dirac equation, such as the Bogoliubov model, are examined and discussed and it is validated that the Dirac equation can provide knowledge about elementary particles.

Sammanfattning

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Chapter 1

Introduction

At the start of the 20th century two new ways to approach physics began being formulated. One of the theories was the theory of relativity which is used when calculating objects at velocities near the speed of light. The other theory was quantum physics, or quantum mechanics, which is used for dealing with physical phenomena at the Planck scale. In quantum physics, the state of a system is described by its quantum state, a state that can be described mathematically as a superposition of vectors in a Hilbert space [1]. A quantum state may change with time, and how it changes can be described by the Schrödinger equation, which is a wave equation. The Schrödinger equation was a great breakthrough in quantum mechanics when it was first formulated in 1925. The Schrödinger equation, while consistent with special relativity, was originally formulated in non-relativistic terms. In order to be able to describe particles at relativistic energy levels we need to adjust the Schrödinger equation.

One of the early attempts at such an adjustment was the Klein-Gordon equation, which indeed is a relativistic version of the Schrödinger equation, but it has some shortcomings. The Klein-Gordon equation was of second order in time and it did not have a positive definite probability density (actually, the indefinite density is not understood to be the probability density, but is understood to be the charge density, which can be both positive and negative) [2].

The Dirac equation was the first ever equation to account fully for both quantum mechanics and special relativity. It was formulated by the British physicist Paul Dirac in 1928. The equation predicts that antimatter must exist, which was unsuspected and unproven at the time of formulation, but has since been proven to exist [3].

In order to avoid the problem of a probability density that was not positive definite, Dirac’s starting point was to try to formulate an equation that should be of first order in both space and time. For that to be possible, he realised that the wave equation must have four components, compared to the Schrödinger equation which has just one component.

Here, the Dirac equation is the main focus, but we will begin with deriving the Klein-
Gordon equation. Then, the Hamiltonian for the Dirac equation in cartesian coordinates will be derived, followed by the Dirac equation in spherical coordinates. The equation is then solved for a particle in a spherical box potential by first solving it for a free particle and then adjusting that solution to the potential. The equation will also be solved numerically and be compared with existing models in which it is used, such as the Bogoliubov model. The last part of the report is a discussion regarding some areas in which the Dirac equation has been applied, such as the MIT bag model.
Chapter 2

Background Material

A quantum state is described by a wave function. Assuming the wave function is a plane wave

$$\psi(x, t) = \psi_0 e^{i(kx - \omega t)}$$  \hspace{1cm} (2.1)

it is possible, using the de Broglie relations $E = h\omega$ and $p = h\mathbf{k}$, to derive the energy operator $\hat{E} \equiv i\hbar \frac{\partial}{\partial t}$ and the momentum operator $\hat{p} \equiv -i\hbar \nabla$. This is described in detail in [4]. From these operators it is straightforward to formulate the Schrödinger equation.

Given a particle in a potential $V(x)$, one can express the total energy for the particle as the sum of the potential energy and the kinetic energy such as

$$E = \frac{1}{2} p^2 + V(x).$$  \hspace{1cm} (2.2)

From this expression, we form the Hamiltonian for the particle by replacing $p$ with the operator $\hat{p}$ which then yields

$$\hat{H} = -\frac{1}{2m} \nabla^2 + V(x).$$  \hspace{1cm} (2.3)

This Hamiltonian represents the total energy of the particle now represented by a wave function. However the energy operator $\hat{E}$ also corresponds to the total energy of the system consisting of one particle. So when these operators act on the wave function we may set them equal. The equation obtained is the famous Schrödinger equation

$$i\hbar \frac{\partial}{\partial t} \psi = -\frac{1}{2m} \nabla^2 \psi + V(x)\psi.$$  \hspace{1cm} (2.4)
2.1 The Klein-Gordon equation

The Schrödinger equation does not take relativistic effects into account due to the non-relativistic Hamiltonian (2.3). Corrections can be made using perturbation theory for both wave functions and energies, the latter will be done in chapter 3.5. Before that, we want to derive and solve a fully relativistic equation, which is achieved using a relativistic energy relation instead of (2.2). Assuming the particle is free, we may utilise the relation between the relativistic energy and momentum $E^2 = m_0^2 c^4 + p^2 c^2$. By substituting with the energy and momentum operators as before and rearranging the equation, we obtain

$$\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 + \frac{m_0^2 c^2}{\hbar^2} = 0. \quad (2.5)$$

By replacing the derivatives with respect to both time and space with the d’Alembertian $\Box = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2$ and then letting it act on the wave function, we get

$$\left( \Box + \frac{m_0^2 c^2}{\hbar^2} \right) \psi = 0. \quad (2.6)$$

This is the famous Klein-Gordon equation [5], which was the first quantum mechanical equation ever suggested that fully took account for special relativity.

However, there were some drawbacks with the Klein-Gordon equation. First, the energies obtained were both negative and positive, which is never the case for the Schrödinger equation for which the energies can never be negative. This was not the biggest problem with the equation, but it meant that what was thought to be the probability density $\rho = \frac{E}{m_0 c^2} |\psi|^2$ [5] could become negative when there were negative energies and was, therefore, not positive definite. A modification and interpretation of this probability density is given in [2].

To get a probability density function similar to the one of the Schrödinger equation, we need to modify the Klein-Gordon equation (2.6).

2.2 Derivation of the Dirac equation

Our derivation of the Dirac equation more or less follows the derivation of the Dirac equation given in [6] combined with a small part from [5].

The problem with the indefinite probability density was caused by the second derivative in time [5]. Therefore, we need to find an equation that commutates with the Klein-Gordon equation, but only with a first derivative with respect to time. A simple way to obtain such an equation is to factorise. To do so, we first define the new operator $\hat{w}$, 

$$\hat{w} = \frac{1}{c^2} \frac{\partial}{\partial t} - \nabla.$$
which squared should equal the d’Alembertian, that is $\hat{\omega}^2 \equiv \Box$. The factorisation of the Klein-Gordon equation (without acting on the wave function) is then

$$
\left( \hat{\omega} + i \frac{m_0 c}{\hbar} \right) \left( \hat{\omega} - i \frac{m_0 c}{\hbar} \right) = 0,
$$

which gives us the following set of equations

$$
\begin{cases}
(\hat{\omega} + i \frac{m_0 c}{\hbar}) \psi = 0 \\
(\hat{\omega} - i \frac{m_0 c}{\hbar}) \psi = 0.
\end{cases}
$$

These equations both satisfy the Klein-Gordon equation while each having fewer solutions [5]. The first equation will be investigated further. To get an explicit expression of the equation, we just need to find $\hat{\omega}$. We assume that $\hat{\omega}$ is of the form

$$
\hat{\omega} = \tilde{\gamma}^\mu \frac{\partial}{\partial x^\mu}
$$

where $\tilde{\gamma}^\mu$ is an unknown operator and $\frac{\partial}{\partial x^\mu}$ is the four-vector representation equal to $(\frac{1}{c} \frac{\partial}{\partial t}, \frac{\partial}{\partial x}, \frac{\partial}{\partial y}, \frac{\partial}{\partial z})$. By substituting (2.9) into the first equation of (2.8), we may rewrite it in Hamiltonian form as

$$
i \hbar \frac{\partial \psi}{\partial t} = \hat{H} \psi = \left( \frac{\hbar c}{i} \left[ \hat{\alpha}^1 \frac{\partial}{\partial x^1} + \hat{\alpha}^2 \frac{\partial}{\partial x^2} + \hat{\alpha}^3 \frac{\partial}{\partial x^3} \right] + \hat{\beta} m_0 c^2 \right) \psi.
$$

Here we have used the notation $\hat{\beta} \equiv (\tilde{\gamma}^0)^{-1}$ and $\hat{\alpha}^i \equiv \hat{\beta} \tilde{\gamma}^i$ for $i \in \{1, 2, 3\}$. We demand that the energy obtained from this equation must still obey the relativistic energy-momentum relation. For this to be true, all eigenfunctions of this slightly modified version of (2.8) must satisfy the Klein-Gordon equation. To impose this condition we square both sides of equation (2.10) and require it to equal the Klein-Gordon equation since, if we succeed, they must commutate. Once squared and ordered by its derivatives, the equation takes on the appearance [6]

$$
-h^2 \frac{\partial^2 \psi}{\partial t^2} = -h^2 c^2 \sum_{i,j=1}^{3} \{\hat{\alpha}^i, \hat{\alpha}^j\} \frac{\partial^2 \psi}{\partial x^i \partial x^j} + \frac{\hbar m_0 c^3}{i} \sum_{i=1}^{3} \{\tilde{\beta}, \hat{\alpha}^i\} \frac{\partial \psi}{\partial x^i} + \beta^2 m_0^2 c^4 \psi.
$$

Here $\{a, b\} = ab + ba$ is the anticommutator. This equation is identical to the Klein-Gordon equation if

$$
\begin{cases}
\{\hat{\alpha}^i, \hat{\alpha}^j\} = 2\delta_{i,j} \\
\{\tilde{\beta}, \hat{\alpha}^i\} = 0 \\
\beta^2 = 1.
\end{cases}
$$

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This is not possible for any scalar, $\tilde{\alpha}^i$, $\tilde{\beta}$ but it is possible if they are quadratic matrices [6] so we assume each one being an $N \times N$ matrix. Because of this, the wave function $\psi$ needs to be a column vector with $N$ components. A detailed derivation of the expression for the matrices $\tilde{\alpha}^i$, $\tilde{\beta}$ is given in [6] and we will simply accept the result yielding

\[
\tilde{\alpha}^i = \begin{pmatrix} 0 & \tilde{\sigma}_i^2 \\ \tilde{\sigma}_i^2 & 0 \end{pmatrix}, \quad \tilde{\beta} = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}.
\] (2.13)

Here, $\tilde{\sigma}_i^2$ are the two-dimensional Pauli matrices [7] and $\mathbb{1}_2$ is the two-dimensional identity matrix. To prevent any ambiguities interpreting the notation in these equations, we present the expression of $\tilde{\alpha}^1$ as an example

\[
\tilde{\alpha}^1 = \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.
\] (2.14)

The wave function, also consisting of four elements, is said to be made up out of two spinors, $\psi_A$ and $\psi_B$, each one containing two elements. That is

\[
\psi = \begin{pmatrix} \psi_0 \\ \psi_1 \\ \psi_2 \\ \psi_3 \end{pmatrix} = \begin{pmatrix} \psi_A \\ \psi_B \end{pmatrix} \quad \text{where} \quad \psi_A = \begin{pmatrix} \psi_0 \\ \psi_1 \end{pmatrix}, \psi_B = \begin{pmatrix} \psi_2 \\ \psi_3 \end{pmatrix}.
\] (2.15)

In the rest of this text we will not be using the four element representation of operators and the wave function but rather the spinor one.

Finally, by making use of the notation $\tilde{\alpha} = \tilde{\alpha}^1 \mathbf{x}_1 + \tilde{\alpha}^2 \mathbf{x}_2 + \tilde{\alpha}^3 \mathbf{x}_3$, where $\mathbf{x}_i$ being the unit vectors in the cartesian coordinate system, we may rewrite the Hamiltonian of the Dirac equation (2.10) in the more compact way

\[
\hat{H} = -i\hbar c \tilde{\alpha} \cdot \nabla + \tilde{\beta} m_0 c^2 = c\tilde{\alpha} \cdot \hat{p} + \tilde{\beta} m_0 c^2,
\] (2.16)

where $\tilde{\alpha} \cdot \hat{p}$ is the kinetic energy operator [7] and $\tilde{\beta} m_0 c^2$ is the rest mass energy operator. If we square both sides of (2.16) we can see great similarities to the relativistic energy-momentum relation.

The probability density function for the Dirac equation will not be derived here, but it is expressed the same way as the Schrödinger equation, $\rho = |\psi|^2$. In the case of the Dirac equation the wave equation is a vector and we can then express $\rho$ as a scalar product, $\rho = \psi^\dagger \cdot \psi$.

To this Hamiltonian we can add a potential. This can be done in several different ways, unlike the Schrödinger equation, where the potential can only be in one certain way.
This is because we now have a four-dimensional equation and the Schrödinger equation is one-dimensional. For a scalar potential, for example, the potential could be either $\mathbb{1}_4 V(x)$ or $\tilde{\beta} V(x)$. The first of these two would then correspond to a potential that relate directly to the energy eigenvalues, since [6]

$$\left(\hat{H} - V(x)\right) \psi = \left(c\tilde{\alpha} \cdot \hat{p} + \tilde{\beta} m_0 c^2\right) \psi. \quad (2.17)$$

The other possible potential would instead affect the rest mass energy

$$\hat{H} \psi = \left(c\tilde{\alpha} \cdot \hat{p} + \tilde{\beta} \left(m_0 c^2 + V(x)\right)\right) \psi. \quad (2.18)$$

This can be described as having a varying rest mass $m(x)$, which you can see an example of in [8].

The first potential is of interest when, for example, we are calculating the states of electrons, because we then are using a Coulomb potential [9]. The second potential can be used to confine a Dirac particle in a specific region [8], and because of this, we will use the second potential throughout the report [5].
Chapter 3

Investigation

3.1 Problem

We want to solve the Dirac equation for a spherical box potential. In order to do that, we must first rewrite the Dirac equation from its cartesian form to its radial form. We will then find the solutions to the Dirac equation for our spherical box potential. The Schrödinger equation and its relativistic correction is then examined for the same potential. At the end of Chapter 3 we examine the concept of bag models and especially the Bogoliubov model.

A spherically symmetric potential is a potential that depends only on the distance between the affected particle and a defined center point. The problem of a particle in a spherically symmetric potential is an important problem in quantum mechanics. Here, we will show how solving the Dirac equation for a spherical box potential can be used to approximate the radius of a nucleon with the help of the Bogoliubov model.

The spherical box potential we will use is [9]

\[ V(r) = \begin{cases} 0 & r < R \\ V_0 & r > R, \end{cases} \]  

(3.1)

where we will let \( V_0 \to \infty \) when examining the bag models. The ramification of this is that any particle inside the spherical box can never leave it.

Bag models were first formulated in the late 1960s when people started suggesting that, since no free quarks had been found, that quarks must be confined within the hadrons in which it had been confirmed that quarks exist. The bag model we will examine is the Bogoliubov model, which is the first and one of the simpler bag models. The model basically describes the three quarks that exist inside a hadron as three particles affected by our potential (3.1), which is a bit crude but the model has been shown to give fairly accurate results.
3.2 The Dirac equation in spherical coordinates

Since this problem is spherically symmetric ($V(x) = V(r)$), we would like to work in a spherical coordinate system. Therefore, we need to transform the Hamiltonian of the Dirac equation (2.18) from cartesian coordinates to spherical coordinates. This is done in great detail in [7], which we will follow.

To begin with, we may express the nabla operator as [7]

$$\nabla = \hat{r} (\hat{r} \cdot \nabla) - \hat{r} \times \hat{r} \times \nabla = \hat{r} \frac{\partial}{\partial r} - \frac{i}{\hbar} \hat{r} \times \hat{L},$$

where we have used $\hat{L} = \hat{r} \times \hat{p}$. Here, $\hat{r} = \hat{r}(\theta, \phi)$ is the unit radial vector and $r = |\mathbf{r}|$ is the distance to the origin. By substituting this into the relativistic kinetic energy operator, we obtain

$$\hat{\alpha} \cdot \hat{p} = -i\hbar \hat{\alpha} \cdot \hat{r} \frac{\partial}{\partial r} - \hat{\alpha} \cdot \hat{r} \frac{\hat{L}}{r}.$$  (3.3)

To be able to proceed, we first need four new matrices, the four-dimensional Pauli matrices $\tilde{\sigma}^i$, and the $\tilde{\gamma}^5$-matrix. The new Pauli matrices are defined in a similar manner to the $\tilde{\alpha}^i$ of equation (2.13) but having the $\tilde{\sigma}_2^i$ on the diagonal rather than the anti-diagonal. The $\tilde{\gamma}^5$-matrix is defined by $\tilde{\gamma}^5 \equiv i\tilde{\gamma}^1\tilde{\gamma}^2\tilde{\gamma}^3\tilde{\gamma}^4$ [7] where the $\tilde{\gamma}^\mu$ is the ones used in equation (2.9). For clarity, we present the matrices

$$\tilde{\sigma}^i = \begin{pmatrix} \tilde{\sigma}_2^i & 0 \\ 0 & \tilde{\sigma}_2^i \end{pmatrix}, \quad \tilde{\gamma}^5 = \begin{pmatrix} 0 & -\mathbb{1}_2 \\ -\mathbb{1}_2 & 0 \end{pmatrix}. \quad (3.4)$$

Using the newly defined Pauli matrices, one can show that [7]

$$\tilde{\alpha} \cdot \mathbf{A} \tilde{\alpha} \cdot \mathbf{B} = \mathbf{A} \cdot \mathbf{B} + i\tilde{\sigma} \cdot \mathbf{A} \times \mathbf{B} \quad (3.5)$$

where $\mathbf{A}, \mathbf{B}$ are arbitrary vectors and $\tilde{\sigma} = \tilde{\sigma}^1\hat{x}_1 + \tilde{\sigma}^2\hat{x}_2 + \tilde{\sigma}^3\hat{x}_3$ are similar to $\tilde{\alpha}$. It is possible to form this relation due to the fact that $\tilde{\alpha}$ and $\tilde{\sigma}$ are made up of the two-dimensional Pauli matrices, which have the commutation relations $[\tilde{\sigma}_2^a, \tilde{\sigma}_2^b] = 2i\varepsilon_{abc}\tilde{\sigma}_2^c$, $\{\tilde{\sigma}_2^a, \tilde{\sigma}_2^b\} = 2\delta_{ab}\mathbb{1}_2$. We know that $\hat{r} \perp \hat{L}$, so by setting $\mathbf{A} = \hat{r}, \mathbf{B} = \hat{L}$ and multiplying by $i$ we may simplify (3.5) into

$$i\tilde{\alpha} \cdot \hat{r} \tilde{\alpha} \cdot \hat{L} = -\tilde{\sigma} \cdot \hat{r} \times \hat{L}. \quad (3.6)$$

Furthermore, we can easily find the relations $\tilde{\alpha} \tilde{\gamma}^5 = \tilde{\gamma}^5 \tilde{\alpha} = -\tilde{\sigma}$, $\tilde{\sigma} \tilde{\gamma}^5 = \tilde{\gamma}^5 \tilde{\sigma} = -\tilde{\alpha}$ and $[\hat{r}, \tilde{\gamma}^5] = [\hat{L}, \tilde{\gamma}^5] = 0$. Taking these relations into consideration, we post-multiply (3.6) with $\tilde{\gamma}^5$ and then introduce the $\hat{K}$-operator (A.5) giving us
\[
\hat{\sigma} \cdot \hat{r} \left( \hat{\beta} \hat{K} - \hbar \right) \hat{\gamma}^5 = \hat{\alpha} \cdot \hat{r} \times \hat{L}.
\] (3.7)

Substituting this into the expression for the relativistic kinetic energy operator (3.3) and plugging that into the Dirac Hamiltonian (2.18) yields

\[
\hat{H}(r, \theta, \phi) = i \tilde{c} \tilde{\sigma} \frac{\hbar}{r} \left( \frac{\hbar}{r} - \hat{\beta} \hat{K} \right) \hat{\gamma}^5 + \hat{\beta} \left( m_0 c^2 + V(r) \right).
\] (3.8)

\[\tilde{\sigma} \cdot \hat{r} \] will later be of particular interest to us. Substituting the expression for \(\hat{H}(r, \theta, \phi)\) into the Dirac equation (2.10), we obtain

\[
i\hbar \frac{\partial \psi}{\partial t} = \left[ i \tilde{c} \tilde{\sigma} \left( \frac{\hbar}{r} - \hat{\beta} \hat{K} \right) \hat{\gamma}^5 + \hat{\beta} \left( m_0 c^2 + V(r) \right) \right] \psi
\] (3.9)

which is the Dirac equation in spherical coordinates that we now will solve.

### 3.3 Dirac equation - particle in a spherical box potential

According to [7], the \(\hat{K}\)-operator in appendix A commutates with the Hamiltonian \(\hat{H}\), which can be shown using the relation \(\tilde{\sigma} \tilde{\gamma} = -\chi_m \) (this relation is possible because of the anticommutation relation \([\tilde{\sigma}, \hat{K}] = 0\) where we also use that \([\tilde{\sigma}, \hat{J}^2] = 0\) \([7, 10]\). This means that they share the spatial part of the eigenfunctions \(\psi(x) = (\chi_n^m, \chi_m^m)^T\), which are discussed in appendix A. Since \(\hat{H}\) is independent of time, it is legitimate to assume \(\psi(x, t) = \psi(t)\psi(x)\). Letting the Dirac equation (3.9) act on such a function will simply boil down to forcing \(\psi(t) = e^{-\frac{iE t}{\hbar}}\) \([9]\). Further on we assume

\[
\psi(x) = \left( \begin{array}{c} g(r) \chi_n^m \\ if(r) \chi_m^m \end{array} \right).
\] (3.10)

where \(g(r), f(r)\) are yet to be determined. We will now let the spatial eigenfunction \(\psi(x)\) be acted on by the Dirac equation where the energy operator has been replaced by the energy \(E\). But before doing so, we rearrange the equation a little and observe that \(\hat{\gamma}^5\) will switch the spinors in \(\psi(x)\), as well as contributing with a minus sign, giving

\[
\begin{pmatrix} i (E - m_0 c^2 - V(r)) & 0 \\ 0 & i (E + m_0 c^2 + V(r)) \end{pmatrix} \begin{pmatrix} g(r) \chi_n^m \\ if(r) \chi_m^m \end{pmatrix} = \chi \tilde{c} \tilde{\sigma} \left( \begin{array}{cc} \frac{\partial}{\partial r} + \frac{1}{r} - \frac{\beta r}{c^2} & 0 \\ 0 & \frac{\partial}{\partial r} + \frac{1}{r} + \frac{\beta r}{c^2} \end{array} \right) \begin{pmatrix} g(r) \chi_n^m \\ if(r) \chi_m^m \end{pmatrix}.
\] (3.11)
Calculating both sides of this equation, which is just a little algebra, leads to the following system of equation for $f, g$

\[
\begin{cases}
\hbar c \left( -\frac{\partial}{\partial r} + \frac{\kappa - 1}{r} \right) f_\kappa = \left( E - m_0 c^2 - V(r) \right) g_\kappa \\
\hbar c \left( \frac{\partial}{\partial r} + \frac{\kappa + 1}{r} \right) g_\kappa = \left( E + m_0 c^2 + V(r) \right) f_\kappa.
\end{cases}
\]  

(3.12)

Both of these equations contain $\kappa$, in other words, both $f$ and $g$ depend on $\kappa$ so $f, g \rightarrow f_\kappa, g_\kappa$. Now let us solve for $g_\kappa$ by factoring out $f_\kappa$ from the lower equation to substitute into the upper one. After some simplification and rearranging, we get

\[
\left[ r^2 \frac{d^2}{dr^2} + 2r \frac{d}{dr} + \left( k^2 r^2 - \kappa (\kappa + 1) \right) \right] g_\kappa = 0
\]

(3.13)

where we used a slightly modified relativistic momentum energy relation $p^2 c^2 = E^2 - (m_0 c^2 + V(r))^2$ and the wave vector $k = \frac{p}{\hbar}$. Given the potential (3.1) and assuming a bound state ($E < m_0 c^2 + V_0, E > 0$) [9], we get the wave vectors

\[
\begin{cases}
 k^2_+ = \frac{E^2 - m_0 c^2}{c^2 \hbar^2} > 0 & r < R \\
 k^2_- = -\bar{k}^2_+ = \frac{E^2 - (m_0 c^2 + V_0)^2}{c^2 \hbar^2} < 0 & r > R
\end{cases}
\]  

(3.14)

To begin with, we solve for $r < R$, which in fact is a free particle solution so we do not need to modify equation (3.13). This is the spherical Bessel differential equation with the solution [6]

\[ g_\kappa(r) = a_1 j_\kappa(k_+ r) + a_2 y_\kappa(k_+ r). \]  

(3.15)

Here $j(r)$ and $y(r)$ are the spherical Bessel functions of the first and second kind respectively along with

\[ l_\kappa = l = \begin{cases} 
 \kappa & \kappa > 0 \\
 -\kappa - 1 & \kappa < 0
\end{cases} \]  

(3.16)

However, $y_n(r)$ for $n \in \{0, 1, 2, \cdots \}$ is irregular at the origin, which is not allowed for physical reasons (velocities above the speed of light etc.), so we choose $a_2 = 0$. Now we calculate $f_\kappa$ using the lower equation of (3.12) along with the relation [11]

\[
\frac{\partial j_\kappa(k_+ r)}{\partial r} = k_+ j_{\kappa-1}(k_+ r) - \frac{l_\kappa + 1}{r} j_\kappa(k_+ r) = \frac{l_\kappa}{r} j_\kappa(k_+ r) - k_+ j_{\kappa+1}(k_+ r).
\]  

(3.17)
This is done in great detail in [11] and yields [6]

\[ f_\kappa(r) = a_1 \frac{|\kappa|}{\kappa} \frac{c\hbar k^+}{E + m_0c^2} j_\kappa(k_+ r) \]  

(3.18)

where

\[ \bar{l}_\kappa = \begin{cases} 
\kappa - 1 = l - 1 & \kappa > 0 \\
-\kappa = l + 1 & \kappa < 0.
\end{cases} \]  

(3.19)

For the case \( r > R \), we want to modify equation (3.13) to suit us better. Following [12] one will arrive at the equation

\[ \left[ x^2 \frac{d^2}{dx^2} + x \frac{d}{dx} - \left( x^2 + (\kappa + \frac{1}{2})^2 \right) \right] Z = 0 \]  

(3.20)

with \( x \equiv \bar{k}_- r \) and \( g_\kappa(r) \equiv Z(x)x^{-1/2} \). This is the modified Bessel's equation with solutions \( I_{\kappa+1/2}(x) \) and \( K_{\kappa+1/2}(x) \) known as the modified Bessel functions of first and second kind respectively [13]. Expressed in terms of \( r \), the expression for \( g_\kappa(r) \) becomes [6]

\[ g_\kappa(r) = \sqrt{\frac{2\bar{k}_-}{\pi r}} \left( b_1 I_{\kappa+1/2}(\bar{k}_- r) + b_2 K_{\kappa+1/2}(\bar{k}_- r) \right). \]  

(3.21)

Since \( I_{>0}(r) \) is growing continuously with larger \( r \) and we force \( g_\kappa(\infty) = 0 \), we need to set \( b_1 = 0 \). Again, to calculate \( f_\kappa \), we use the lower equation of (3.12), but now along with the relation [14]

\[ \frac{\partial K_{\kappa+1/2}(z)}{\partial z} = -K_{\kappa-1/2}(z) - \frac{l_\kappa + \frac{1}{2}}{z} K_{\kappa+1/2}(z) \]

(3.22)

\[ = \frac{l_\kappa + \frac{1}{2}}{z} K_{\kappa+1/2}(z) - K_{\kappa+3/2}(z). \]

This then gives the solution [6]

\[ f_\kappa(r) = -b_2 \frac{c\hbar k_-}{E + m_0c^2 + V_0} \sqrt{\frac{2\bar{k}_-}{\pi r}} K_{\kappa+1/2}(\bar{k}_- r). \]  

(3.23)

We finally have all the non-normalised eigenfunctions to the Dirac equation in a spherical potential box. However, for the sake of this report, we will skip the normalisation since we are merely interested in the energy eigenvalue \( E \). We will also only investigate the \( s \)
states, that is, \( l = 0 \Rightarrow \kappa = -1, l_\kappa = 0, \bar{l}_\kappa = 1 \). To do so, we will join \( g_\kappa, g_\kappa' \) at \( r = R \) for the inner and outer solution [9]. For the \( s \) states we have [9, 13]

\[
\begin{align*}
\begin{cases}
    j_0(k_+ r) = \frac{\sin k_+ r}{k_+ r} \\
    K_{1/2}(\bar{k}_- r) = \sqrt{\frac{\pi}{2}} \frac{e^{-k_- r}}{\sqrt{k_- r}}.
\end{cases}
\end{align*}
\] (3.24)

Substituting with these into (3.15) and (3.21) and including the constraint \( a_2 = b_1 = 0 \) whilst using the abbreviation \( x = k_+ R \) and \( y = \bar{k}_- R \), gives us

\[
\begin{align*}
    a_1 &= b_2 \frac{e^{-y}}{R} x \sin x \\
    a_1 &= -b_2 \frac{e^{-y}(y + 1)}{R} \left( \cos x - \frac{\sin x}{x} \right)^{-1}.
\end{align*}
\] (3.25)

By setting these equations equal and then shortening them as much as possible, we end up with [15]

\[
\tan k_+ R = -\frac{k_+}{k_-}.
\] (3.26)

Of particular interest to us is the limit \( V_0 \to \infty \) combined with \( E \gg m_0 c^2 \) meaning we may neglect the rest mass \( m_0 \). This approximation is valid for bound states of light quarks, say \( u \) and \( d \), where the rest mass energy \( m_0 c^2 \) contribution to the total energy \( E \) of the quark is negligible [9]. Using the expressions for the wave vectors (3.14), the quantisation condition (3.26) will decompose into

\[
\begin{align*}
    E_n &= \frac{\pi \hbar c}{R} n, \quad n \in \mathbb{Z}.
\end{align*}
\] (3.27)

This energy relation is linear, which is in good agreement with the approximately linear experimental results [9, 16] (see figure 3.1).

We know that the Dirac equation is in a relativistic framework. The next thing we will do is to try and relate the relativistic results to the results we would get in a non-relativistic framework by examining the Schrödinger equation in a similar manner as we did the Dirac equation. After that, we will compare the relativistic results to the results of a non-relativistic framework with a relativistic perturbation by adding a relativistic correction to the Schrödinger equation.
3.4 Schrödinger equation - particle in a spherical box potential

Let us now try to find a relativistic correction of the Schrödinger equation (2.4) using a similar approach. Just as before, we assume the solution to the wave equation to be of the form $\psi(x, t) = \psi(t)\psi(x)$, and using the same argument as before, we get $\psi(t) = e^{-iEt/\hbar}$. This means that the eigenvalue problem we are to solve is the energy eigenvalue problem (2.3). Since the used potential (3.1) is spherically symmetric, we rewrite the kinetic energy operator into spherical coordinates \[ -\frac{\hbar^2}{2m} \nabla^2 = -\frac{\hbar^2}{2m r^2} \left[ \frac{\partial}{\partial r} \left( r^2 \frac{\partial}{\partial r} \right) - \hat{L}^2 \right] \] (3.28)

where $\hat{L}$ is the orbital angular momentum. $\hat{L}^2$ has the eigenvalues $l(l + 1)$ and the eigenfunctions are the spherical harmonics $Y^m_l(\theta, \phi) = Y^m_l$. Since our potential does not depend on angle, we will assume that the spatial eigenfunctions are of the form $\psi(x) = g(r)Y^m_l$. By plugging into (2.3) and rearranging, we obtain

$$ \left[ r^2 \frac{\partial^2}{\partial r^2} + 2r \frac{\partial}{\partial r} + (k^2 r^2 - l(l + 1)) \right] g_l(r) = 0 $$

(3.29)

where $k^2 = \frac{2m(E - V(r))}{\hbar^2}$. We recognise this equation to be the same as in (3.13). We are only interested in the case $E < V_0$. Just as in (3.14)

$$ \begin{cases} k^2_+ = \frac{2mE}{\hbar^2} > 0 & r < R \\ k^2_- = -\bar{k}^2 = \frac{2m(E - V_0)}{\hbar^2} < 0 & r > R. \end{cases} $$

(3.30)

The only difference between (3.13) and (3.29) is that $\kappa \to l$ and the values of $k^2$; in all other regards they are identical. The solutions can then easily be obtained by replacing $l_\kappa$ with $l$ in (3.15) and (3.21). Just as before, we can show that $a_2 = b_1 = 0$, which gives

$$ g_l(r) = \begin{cases} a_1j_l(k_+ r) & r < R \\ b_2\sqrt{2k_- / \pi r} K_{l+1/2}(\bar{k}_- r) & r > R. \end{cases} $$

(3.31)

As before, the s states are the only states of which we have any interest in. By repeating what we did to get the expression (3.24) and by utilising the fact that both the wave equation and its derivative has to be continuous, we can get the energy eigenvalues. The demands on the wave equation means that $g_0(r \leq R)$ has to be equal to $g_0(r \geq R)$.
when \( r = R \). The same applies for \( g_0'(r \leq R) \) and \( g_0'(r \geq R) \). The counterpart of equation (3.25) for the Schrödinger equation is actually identical, which means that the quantisation condition also remains the same and is given by (3.26). By substituting our new \( k_+, \bar{k}_- \) into our equation and then let \( V_0 \to \infty \), we get for the energy eigenvalues

\[
E_n^{(0)} = \frac{\pi^2 \hbar^2}{2mR^2} n^2, \quad n \in \mathbb{Z},
\]  

(3.32)

where the raised number indicates the order of correction. We can see that the energy eigenvalues relate to \( n \) quadratically, compared to the linear relation to \( n \) of (3.27).

### 3.5 First order relativistic correction

According to [18], the first-order relativistic correction to our Hamiltonian (2.3) is

\[
\hat{H}_{\text{rel}} = -\frac{\beta^4}{8mc^2}.
\]

The total Hamiltonian is then \( \hat{H}^{(1)} = \hat{H}^{(0)} + \hat{H}_{\text{rel}} \) where the raised number indicates the order of correction as usual. The Hamiltonian \( \hat{H}^{(0)} \) is the Hamiltonian for the Schrödinger equation (2.3). As a result of \( \hat{H}_{\text{rel}} \), we will get a correction to our energy, \( E_{\text{rel}} \). If we assume that the correction \( E_{\text{rel}} \) is significantly smaller than the energies we get from \( \hat{H} \), then we can use time-independent perturbation theory. In the case of s states, the energies are not degenerated; see (3.32). We can then write the relativistic energy correction in bra-ket notation as

\[
E_{\text{rel}} = \langle nlm|\hat{H}_{\text{rel}}|nlm\rangle = -\frac{1}{2mc^2}\langle nlm|\hat{H}^2 + 2V(r)\hat{H} + V(r)^2|nlm\rangle
\]

\[
= -\frac{1}{2mc^2}\left( E_n^2 + 2E_n\langle V(r) \rangle + \langle V(r)^2 \rangle \right).
\]

(3.33)

We already know that when we let \( V_0 \to \infty \) it will cause \( K_{1/2}(\bar{k}_-r) \to 0 \), which means that \( g_0(r > R) \equiv 0 \). Consequently, \( \langle V(r)^s \rangle = 0 \). By inserting this into (3.33), we get

\[
E_{\text{rel}} = -\frac{E_n^2}{2mc^2}
\]

(3.34)

The relativistically corrected energy can now be obtained by \( E_n^{(1)} = E_n^{(0)} + E_{\text{rel}} \) and by inserting our expression for \( E_{\text{rel}} \), we get the relativistically corrected energy

\[
E_n^{(1)} = E_n^{(0)} - \frac{E_n^{(0)^2}}{2mc^2} = \frac{\pi^2 \hbar^2}{2mR^2} n^2 - \frac{\pi^4 \hbar^4}{8m^3 c^2 R^4} n^4.
\]

(3.35)
3.6 Bogoliubov model

A hadron is a composite particle consisting of quarks held together by the strong force. A hadron either consists of three quarks (or three anti-quarks) or one quark and one anti-quark. We will examine protons and neutrons, which are hadrons consisting of three quarks with a spin of 1/2. Hadrons with half-spin integers are called baryons, and baryons are fermions [19].

Quarks have a property called color charge. A hadron must have zero total color charge due to a phenomena called color confinement [20]. This restraint can be reproduced, though not perfectly, by bag models. In a bag model we consider the hadron to be a bag, e.g. a spherical well with infinitely high walls that contain the quarks that make up the hadron. This approximation is possible due to the strong force holding the quarks together. The strong force is weak when the quarks are very close to each other (inside the hadron) but becomes very strong when they get further apart (at the walls of the well).

One of the simpler bag models is called the Bogoliubov model. The Bogoliubov model can be considered to be a quantum mechanical bag for which, if we solve the Dirac equation within the bag, will provide useful knowledge of the properties of elementary particles. The model imagines the hadron to be a spherical well with the potential (3.1) [15]. This potential is the same that we used to solve the Dirac equation in Chapter 3.3, and hence we know the energy eigenvalues for the quarks (3.27). We now assume, due to the strong force, that the quarks inside the hadron can be considered as three non-interacting particles all of which are unable to ever leave the bag [15]. The energy of the hadron is then the sum of the energy of the quarks. We know that two identical fermions can not share the same quantum state according to the Pauli exclusion principle. However, the color property of the quark actually makes them non-identical, since the quarks in a baryon do not share the same color, and hence we do not break the Pauli exclusion principle even when all the quarks share the same energy state [21].

By fitting the energy quantisation condition (3.27) to the experimental values of the nucleus, we can get an optimal theoretical value for the radius, which we then can compare to the experimental value. Below is a table comparing the theoretical value of the mass of the spin-1/2 nucleon for the Dirac equation \(m_{DE}\) to the experimental values of the mass of the nucleon \(m_{exp}\) for the seven lowest energy states, where \(n\) describes which energy state each particle is in.

<table>
<thead>
<tr>
<th>(n)</th>
<th>(m_{DE})</th>
<th>(m_{exp})</th>
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<tbody>
<tr>
<td>1</td>
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</table>
Table 3.1: $m_{\text{exp}}$ are the experimental values of the spin-1/2 nucleons mass, while $m_{\text{DE}}$ are the theoretical values predicted by our model for the Dirac equation after a one-parameter fit. The optimal value of $R = 2.35 \text{[fm]}$ gives us a model mean error of 11.8%.

The actual value of the radius of the neutron is $\approx 0.85/\text{[fm]}$. Comparing this to the expected value of the radius, which in the case of the Dirac equation can be expressed as $\langle r \rangle \approx 3R/4 \approx 1.76 \text{[fm]}$ [15], we see that our value is quite good given the crudeness of the model. However, the error varies significantly, which could indicate that we are a bit lucky to have a theoretical value which is as close as it is to the experimental value.

We will now repeat the above process for the Schrödinger equation and its first-order relativistic correction. We will fit our quark mass and quark radius so that our energy eigenvalues will get as close to the experimental energy values as possible. We can then compare the predicted quark mass and nucleon radius of our model to the experimental values of $m_q$ and the nucleon radius. Below is the table comparing the experimental values to the Schrödinger equation having done a two-parameter fit for $m_q$ and $R$, though for the Schrödinger equation it is possible to do a one-parameter fit if the parameter we fit is $m_q R^2$.

Table 3.2: Theoretical values of the Schrödinger equation with a two-parameter fit to experimental data [16] for spin-1/2 nucleon masses. The optimal value of $R = 15.7 \text{[fm]}$ and the optimal value of $m_q = 7.83 \text{[MeV/c^2]}$ gives a mean error of 32.8%.

We see that the value of the radius is not nearly as good as for the Dirac equation, but the mass of a quark is considered to be in the range of 1.7-5.7 [MeV/c^2] [22], which means that our fitted $m_q$ is really close to the actual value. The mean error is still fairly low, but just as before, the credibility of the mean error is significantly diminished by how much the error varies.

Doing the same for the first order relativistically corrected energies of the Schrödinger equation, we acquire the values in the table below.
\begin{table}[h]
\centering
\begin{tabular}{|c|c|c|c|c|c|c|c|c|}
\hline
$n_{q_1}, n_{q_2}, n_{q_3}$ & 1,1,1 & 2,1,1 & 2,2,1 & 2,2,2 & 3,2,2 & 3,3,2 & 3,3,3 \\
\hline
$m_{\text{exp}}$ [MeV] & 940 & 1440 & 1535 & 1650 & 1710 & 2090 & 2100 \\
\hline
$m_{\text{RCSE}}$ [MeV] & 629 & 1057 & 1484 & 1912 & 1955 & 1998 & 2041 \\
\hline
Error & 33.1\% & 26.6\% & 3.29\% & 15.9\% & 14.3\% & 4.41\% & 2.82\% \\
\hline
\end{tabular}
\caption{Theoretical values of the first order relativistically corrected Schrödinger equation with a two-parameter fit to experimental data \cite{16} for spin-1/2 nucleon masses. The optimal value of $R = 0.745$ [fm] and the optimal value of $m_q = 1530$ [MeV/c$^2$] gives a mean error of 14.4\%.
}
\end{table}

For the relativistically corrected Schrödinger equation we get a really good R that is in the correct order of magnitude. However, the fitted quark mass is around 300 times larger than the actual value of the quark mass, which makes these results the least credible. The error is a lot smaller for the first order relativistically corrected Schrödinger equation than for the non-relativistic one, and the error does not vary as greatly, which is due to that that for the relativistically corrected equation we can vary two variables, but for the non-relativistic version we can only vary $m_q R^2$ as one variable.

The tables presented above have been plotted in figure 3.1 below in order to easily compare them to the experimental data. We can see that the plot of the two-parameter fitted Dirac equation overlaps the plot of the one-parameter fitted version which we will discuss below. We also observe that the plot for the Dirac equation has a shape more similar to the imaginable curve for the experimental data than either of the plots for the Schrödinger equation, and the fact that the experimental data can be approximated as linear is clear. The Schrödinger equation has quite poor values, and we can see that for the uncorrected Schrödinger equation the curve is nowhere near the experimental data. For the relativistically corrected Schrödinger equation the curve is actually quite good in comparison to the experimental values, but the fitted value for $m_q$ is off by such a large margin that we can not trust the perturbed version.

\section{Discussion}

The optimal value of the radius of the nucleus for the Dirac equation using the Bogoliubov model was close to the actual value of the radius of the nucleus, which suggests that our approximations for the Dirac equation were valid. One of the approximations we made was that $E^2 \gg m_0^2 c^4$, so that we could neglect the rest mass $m_0$. If we had not neglected the rest mass our energy quantisation condition (3.27) would instead have been

\[
E_n = \sqrt{m_0^2 c^4 + \left(\frac{\pi \hbar c}{R} n\right)^2}, \quad n \in \mathbb{Z}.
\]

(3.36)
Figure 3.1: Experimental [16] and fitted theoretical values for spin-1/2 nucleon masses. The 0 on the x-axis corresponds to the ground state, and then it counts up, e.g. the 6 corresponds to the sixth excited state.

By making a two-parameter fit to the experimental data the same way we did the one-parameter fit for the Dirac equation when the only unknown was $R$, we get the exact same table as in 3.1 which means that the optimal radius is still $R = 2.35 \text{ fm}$. However, we also have a value for $m_0 = m_q = 7.23[\text{MeV}/c^2]$, which is close to the real value of $m_q$. This validates the assumption that $E^2 \gg m_0^2c^4$. In figure 3.1, $m_{DE,m_q}$ has been plotted as well, and as we can see it overlaps the plot of $m_{DE}$.

For the Schrödinger equation, the values were not as good as for the Dirac equation, but they were not so far off that they should be disregarded. However, for the relativistically corrected Schrödinger equation, the value of $m_q$ was far off, being around 300 times larger than the experimental values. This suggests that getting a relativistic correction by perturbation theory might not be valid here, so we are interested in the ratio between $E_{rel}$ (3.32) and $E_n$ (3.34). We get the following

$$\left| \frac{E_{rel}}{E_n^{(0)}} \right| = \frac{E_n^{(0)}}{2mc^2} = \left( \frac{\pi \hbar}{2mcR} \right)^2 n^2 \approx 9700 n^2 \quad (3.37)$$
where we have used the experimental data \( m = \langle m_q \rangle = 3.7 \, [\text{MeV}/c^2] \) and \( R = 0.85 \, [\text{fm}] \).

When we apply perturbation theory we assume that our corrections will be much smaller than our non-perturbed energies. In this case the relativistic correction is 9700 times larger for the ground state, given that the model uses the correct values for the radius and quark mass, which is the only case we are interested in, and then it grows quadratically with \( n \). This means that our relativistic corrections are much greater than our non-corrected energies and hence the assumption we made when we applied perturbation theory is not correct and we conclude that the usage of perturbation theory is not valid here.

That perturbation theory is not valid here is not unexpected. We assumed in our relativistic correction that \( p^2c^2 \ll m^2c^4 \), and then Taylor-expanded for small \( p \). In our case, though, the experimental data suggests that \( p^2c^2 \) is not so small compared to \( m^2c^4 \), so our Taylor-expansion is not justified. For the Dirac equation we assumed that \( E \gg m_0c^2 \) which is equivalent to \( pc \gg 0 \) which the experimental data confirmed was a good approximation. This also suggests that the assumption \( p^2c^2 \ll m^2c^4 \) is not valid.

We can conclude that the Dirac equation more accurately predicts the attributes of elementary particles than the Schrödinger equation if we use Bogoliubovs bag model. This is expected since Bogoliubov had the Dirac equation in mind when he first thought of the concept of bag models.

The Bogoliubov model is very simple and crude and there are more precise models. One of the most favored models is the MIT bag model. The MIT bag model describes particles as composite systems with their internal structure being associated with quark and gluon field variables, and it utilises boundary conditions that are consequences of color confinement coupled with solving the Dirac equation for a free particle.

The MIT bag model addresses very complicated problems in quantum field theory. For practical purposes, it has mainly been used in a much simpler form where the cavity is taken to be a static, spherical cavity of radius \( R \), fixed by satisfying a boundary conditions on average over the surface of the bag. This is actually the model of Bogoliubov but with the radius determined dynamically. To learn more about the MIT bag model we suggest reading [23], which is at the time of writing a work in progress, but that should be available to the public by the time this report is.
Chapter 4

Summary and Conclusions

We have examined the Dirac equation for a spherical box potential. This is done by first rewriting the Dirac equation into spherical coordinates. We then solved the Dirac equation for a particle affected by a spherical box potential in the spherical coordinate system and found the energy eigenvalues of the equation. These eigenvalues were then used to estimate the radius of a nucleus by using the Bogoliubov model. The eigenvalues were linear, which is in good agreement with the experimental data, which is approximately linear. This is not the case for the Schrödinger equation or the relativistically corrected version of it, where the eigenvalues are quadratic and quartic respectively. This suggests that the Bogoliubov model is better suited for the Dirac equation than either of the two versions of the Schrödinger equation.

The estimated value of the radius was close to the actual value which suggests that the Bogoliubov model works well for the Dirac equation. The same thing was done for the Schrödinger equation and a relativistically corrected version of the Schrödinger equation, and we concluded that the Bogoliubov model did not predict as good of values for either of the two as it did for the Dirac equation. The results of the relativistically corrected version of the Schrödinger equation was much worst than for the non-relativistic Schrödinger equation. The main reason that the Bogoliubov model does not work well for the relativistically corrected Schrödinger equation is the fact that the corrected version was acquired using perturbation theory. Perturbation theory assumes the relativistic energy corrections to be much smaller than the non-relativistic energies. In our case the relativistic corrections were far greater than the non-relativistic energies which means that perturbation theory should not be applied.

We also mentioned above that the experimental data is approximately linear, which is not the case for either of the two Schrödinger equations. For the non-relativistic Schrödinger equation the eigenvalues are quadratic, and for the relativistically corrected Schrödinger equation they are quartic. This also suggests that the Dirac equation is better suited for the Bogoliubov model.
Appendix A

The $\hat{K}$ Operator

This appendix is a short summary of the most important steps from [7, 24] for deriving the spherical Dirac Hamiltonian (3.9) as well as a motivation of the assumption made regarding its eigenfunctions.

A.1 The two-dimensional $\hat{K}_2$ operator

Defining the operator

$$\hat{K}_2 = \hat{\sigma}_2 \cdot \hat{\mathbf{L}} \cdot \hbar + \frac{1}{\hbar} \left( \hat{J}^2 - \hat{L}^2 \right) + \frac{1}{4} \hbar$$

(A.1)

in which we have used the relation

$$\hat{J}^2 = (\hat{S} + \hat{\mathbf{L}})^2 = \hat{S}^2 + 2\hat{S} \cdot \hat{\mathbf{L}} + \hat{\mathbf{L}}^2 = \hbar \hat{\sigma}_2 \cdot \hat{\mathbf{L}} + \frac{3}{4} \hbar^2.$$ (A.2)

Substituting with the eigenvalues for $\hat{J}^2$ and $\hat{\mathbf{L}}^2$ one finds that the eigenvalues for this operator may be written as $-\hbar \kappa$ where

$$\kappa = \begin{cases} -l - 1 < 0 & j = l + \frac{1}{2} \\ l > 0 & j = l - \frac{1}{2} \end{cases}.$$ (A.3)

From this, it is obvious that the sign of $\kappa$ determines the value of $j$ and that the magnitude of $\kappa$ determines the value of $l$. If we, in the remaining calculations, replace the quantum numbers $j$ and $l$ with the quantum number $\kappa$, the calculations will become easier to do, which is why we make the substitution.
A.1.1 Eigenfunctions

The eigenfunctions to the $\hat{L}^2, \hat{L}_z$ and $\hat{S}^2, \hat{S}_z$ operators are the spherical harmonics $Y_l^m(\theta, \phi) = Y_l^{m\kappa}$ and 1/2-spinors $\chi^m = \chi_\pm$ respectively. Because these quantities exist in different subspaces, and therefore commute, the collective eigenfunctions amongst all of these operators are simply the direct product between the spherical harmonics and 1/2-spinors $Y_l^m \otimes \chi_\pm$. For simplicity, we will in further appearances ignore the $\otimes$, however the product between the eigenfunctions should still be understood as direct product.

One can show that the set of operators $\hat{K}_2, \hat{J}^2, \hat{L}^2, \hat{S}^2, \hat{J}_z$ mutually commute. However, $\hat{J}^2$ does not commute with any of $\hat{L}_z, \hat{S}_z$. Thus, the set of operators specified above and the set of operators $\hat{L}^2, \hat{S}^2, \hat{L}_z, \hat{S}_z$ form their own basis. The eigenfunctions to the first set of operators are known as the spin-angular functions $\mathcal{Y}_l^j$. These eigenfunctions may be represented as a linear combination of the $Y_l^m \otimes \chi_\pm$ using the Clebsch-Gordon coefficients. However, these coefficients are equal to zero unless the conditions $m = m_l + m_s$ and $|l - s| \leq j \leq l + s$ are fulfilled. For our case, where $m_s = \pm s = \pm \frac{1}{2}$, these conditions reduce to $m = m_l \pm \frac{1}{2}$ and $j = l \pm s$ respectively. So the spin-angular may therefore be written as

$$
\begin{align*}
\mathcal{Y}_l^j = & \left( l, \frac{1}{2}; m - \frac{1}{2}, \frac{1}{2} \right| l, \frac{1}{2}, l \pm \frac{1}{2}, m \left| Y_l^m \chi_+ \right.
\end{align*}
$$

where, $| \cdots | \cdots$ being the Clebsch-Gordon coefficients, which are found in [7] table 2.2. Replacing the $j$ and $l$ quantum number with $\kappa$ we may represent both of (A.4) with $\chi_\kappa^m \equiv \mathcal{Y}_l^{j,m}$. Whether $j = l \pm \frac{1}{2}$ is determined by the sign of $\kappa$ according to (A.3).

A.2 The four-dimensional $\hat{K}$ operator

According to [7], we form the four-dimensional $\hat{K}$ operator as

$$
\hat{K} = \hat{\beta} \left( \hat{\sigma} \cdot \hat{L} + \hat{h} \right) = \hat{\beta} \otimes \hat{K}_2 = \begin{pmatrix} \hat{K}_2 & 0 \\ 0 & -\hat{K}_2 \end{pmatrix}.
$$

where, $\otimes$ is the Kronecker product [25]. By using the known eigenfunctions of $\hat{K}_2$, we may create the eigenfunctions of this operator by inspection. If defining them $(\chi_\kappa^m, \chi_{-\kappa}^m)^T$, the eigenvalue becomes $-\hbar \kappa$ where $\kappa$ is the same as in (A.3). The only difference in the original quantum numbers $j, l$ and $m$ between $\chi_\kappa^m$ and $\chi_{-\kappa}^m$ is that $l$ differ by one [10].
References


[23] Lagerkvist L, Samuelsson F. The MIT bag-model; [work in progress].
