KWAME NKRUMAH UNIVERSITY OF SCIENCE AND TECHNOLOGY,

KUMASI

COLLEGE OF SCIENCE

THE DYNAMICS OF KLEIN-GORDON EQUATION FOR A SLOW VARYING INTERACTING WAVE FIELD

A Thesis submitted to the Department of Mathematics, in partial

fulfillment of the requirements for the Degree of



SAPS

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By

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DECLARATION

I hereby declare that this is my own work towards the Master of Philosophy (MPhil) and that, to the best of my knowledge, it contains no material previously published by another person nor material which has been accepted for the award of other degree of the University, except where due acknowledgement has been made in the text.



ABSTRACT

The main purpose of the study was to investigate the outcomes when an interacting term is incorporated into a Klein-Gordon equation, in particular when the interacting term involves a slow periodic wave field. The study further seeks to investigate in the context of Dirac approach to the quantum relativistic free particle. A slow varying periodic field was considered in the study as a potential field which interacted with quantum mechanics wave particle field as in the Schrodinger equation for a forced particle. In the relativistic context of the study, the Klein-Gordon equation was considered as a homogenous differential equation which represented a free particle and the interacting term was placed on the right hand side, having a "slow varying potential" field as a factor.

It was found that for the zeroth order approximation of the slow varying wave field, Klein-Gordon equation still remained as field but there was only a shift in the energy mass. However, with the second order approximation, a formal Quantum Harmonic Oscillator was obtained. This yielded discrete positive and negative energy mass, suggesting particle and antiparticle states.

An equivalent Dirac formalism which also incorporated an interacting term was obtained, with a recovery of particle and antiparticle states by means of creation and annihilation operators.

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DEDICATION

To my lovely wife, Mrs. Matilda Odoom.



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Chapter One

Introduction

1.1 Background

1.1.1 The origins of Quantum Theory

Until the end of the nineteenth century, classical physics appeared to be sufficient to explain all physical phenomena. The universe was conceived as containing matter, consisting of particles obeying Newton's laws of motion and radiation (waves) following Maxwell's equations of electromagnetism. The theory of special relativity, formulated by A. Einstein in 1905 on the basis of a critical analysis of the notions of space and time, generalized classical physics to include the region of high velocities. In the theory of special relativity, the velocity c of light plays a fundamental role: it is the upper limit of the velocity of any material particle. Newtonian mechanics became an accurate approximation to relativistic mechanics only in the non-relativistic regime, that is, when relevant particle velocities were small with respect to c. It should be noted that Einstein's theory of relativity did not modify the clear distinction between matter and radiation which was at the root of classical physics. Indeed, all pre-quantum physics, non-relativistic or relativistic, are now often referred to as classical physics.

During the late nineteenth century and the first quarter of the twentieth century, however, experimental evidence accumulated which came up with new concepts radically different from those of classical physics. Some of them are the

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quantization of physical quantities such as energy and angular momentum, the particle properties of radiation and the wave properties of matter. These concepts were directly related to the existence of a universal constant, called Planck's constant h. Thus, just as the velocity c of light plays a central role in relativity, so does Planck's constant in quantum physics. Because Planck's constant is very small when measured in microscopic units (such as SI units), quantum physics essentially deals with phenomena at the atomic and subatomic levels.

According to Messiah (1958), quantum mechanics is a mode of calculation which purports to explain all physical phenomena, both on an atomic and on a macroscopic scale.

Merzbacher (1973) also defined quantum mechanics as the theoretical framework within which it has been found possible to describe, correlate and predict the behaviour of a vast range of physical systems from elementary particles, through nuclei atoms and radiations, to molecules and solids.

Quantum mechanics is a fundamental physical theory which extends and corrects classical Newtonian mechanics, especially at the atomic and subatomic levels. It takes its name from quantum (that is, for "how much") used in physics to describe the smallest discrete increments into which something is subdivided.

Quantum mechanics describes with great accuracy and precision many phenomena where classical mechanics drastically fails to agree with experiments, including the behavior of systems of very small objects typically the size of atoms or smaller, but also some 'macroscopic' phenomena, like superconductivity and superfludity. Quantum mechanics successfully addresses these failures, achieving unprecedented precision in its agreement with experiment. It also satisfies Correspondence principle, in that it agrees with classical mechanics for those phenomena where classical mechanics agrees with experiment.

Quantum mechanics has had enormous success in explaining many of the features of our world. The individual behavior of the microscopic particles that make up all forms of matter - electrons, protons, neutrons, and so forth - can often only be satisfactorily described using quantum mechanics.

Quantum mechanics is important for understanding how individual atoms combine to form chemicals. The application of quantum mechanics to chemistry is known as quantum chemistry. Quantum mechanics can provide quantitative insight into chemical bonding processes by explicitly showing which molecules are energetically favorable to which others, and by approximately how much. Most of the calculations performed in computational chemistry rely on quantum mechanics.

Much of modern technology operates at a scale where quantum effects are significant. Examples include the laser, the transistor, the electron microscope, and magnetic resonance imaging. The study of semiconductors led to the invention of the diode and the transistor, which are indispensable for modern electronics.

Newtonian mechanics consisted of Kinematics (Special relativity) and Dynamics (Quantum mechanics. Quantum mechanics also comprised of the non-relativistic, which has to do with the development of the Schrodinger equation and relativistic mechanics, which is also in relation to the Klein-Gordon and Dirac equations. When quantum mechanics was originally formulated, it was applied to models whose correspondence limit was non-relativistic classical mechanics. For instance, the well-

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known model of the quantum harmonic oscillator uses an explicitly non-relativistic expression for the kinetic energy of the oscillator, and is thus a quantum version of the classical harmonic oscillator.

Early attempts to merge quantum mechanics with special relativity involved the replacement of the Schrödinger equation with a covariant equation such as the Klein-Gordon equation or the Dirac equation. While these theories were successful in explaining many experimental results, they had certain unsatisfactory qualities stemming from their neglect of the relativistic creation and annihilation of particles. A fully relativistic quantum theory required the development of quantum field theory, which applies quantization to a field rather than a fixed set of particles. The first complete quantum field theory, quantum electrodynamics, provides a fully quantum description of the electromagnetic interaction.

1.2 Statement of the Problem

This study seeks to revisit the homogenous Schrodinger equation, homogenous Klein-Gordon equation and the non-homogenous Schrodinger equation, coming out with their various equations and solutions available. It also seeks to investigate thoroughly the non-homogenous Klein-Gordon equation, when the right hand side of the free particle Klein-Gordon equation is replaced with a forced term, which represents the slow varying wave field. The study would also investigate whether there is a similarity between the non-relativistic free particle Schrodinger equation and the relativistic free particle Klein-Gordon equation. For instance, the non-homogenous Schrodinger and the Klein-Gordon equations are given respectively as

$$\Rightarrow \nabla^2 \psi + \frac{2m}{\hbar^2} E \psi = 0 \dots 1.1b$$

If equations (1.1b & 1.2) are compared, we can literally equate the Laplacian ($\nabla^2 \Psi$) and the D'Alembertian operator ($\Box^2 \Psi$). In addition, the study would investigate the possible solutions to the energy levels with respect to the non-homogenous Klein-Gordon equation. It will again probe into the existence of the creation and annihilation eigenvalues and eigenfunctions of the non-homogenous Klein-Gordon equation by application of the Dirac format.

1.3 Objectives

The objectives of the study are as follow:

To review the homogeneous Schrodinger equation, homogenous Klein-Gordon equation and the corresponding Dirac Equation.

To study the non-homogeneous Klein Gordon equation with a slow varying wave as the interacting term on the Right Hand Side.

1.4 Methodology

The study looked at a free particle Schrodinger equation as a homogenous differential equation. A potential field interacting with a wave function field was replaced at the right hand side of the homogenous equation. The free particle Klein-Gordon equation was also considered. With this equation, a forced term which represents a slow varying wave field reacted with the wave function field on the right hand side of the free Klein-Gordon equation, making it non-homogenous. Both the zero order and the second order terms of the slow varying wave field became the interacting terms. Finally, the non-homogenous Klein-Gordon was also solved using the Dirac format.

1.5 Organization of the study

The study is organized into five chapters. Chapter one deals with the introduction. This consists of the background which contains the origins to quantum theory, the statement of the problem, objectives, methodology and the organization of the study. Chapter two also deals with the review of literature. In it, we have the review of the non-relativistic quantum mechanics, the interpretation of Schrodinger equation: continuity equation, solutions to the non-homogenous Schrodinger equation, negative energies and antiparticle of Schrodinger equation. Chapter three also contains the review of the relativistic quantum mechanics, which also contains the definition relativistic quantum mechanics, Minkowski's space, four-vectors, the fourvelocity, and the relationship between proper time and an ordinary time. It has also been organized under the following sub-headings: review of the Hamiltonian and Klein-Gordon equation, interpretation of Klein-Gordon equation: continuity equation, Fourier expansion and momentum space of Klein-Gordon equation, review of Dirac equation, probability and current for Dirac equation, positive energy and antiparticles, free particle solution. Simple solutions: non-relativistic approximations. The main results were treated in chapter four, which contains the non-homogenous Klein-Gordon equation with the interacting term. It is organized under the following sub- headings: slow varying wave field, effects of slow varying wave field on the Schrodinger equation, effects of the slow varying wave field on the Klein-Gordon

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equation, Dirac equation, and the annihilation and creation operators whilst chapter five focuses on the summary of results, conclusions and the recommendations.



Chapter Two

The Review of Non-Relativistic Quantum Mechanics

This chapter is aimed at reviewing the non-relativistic quantum mechanics, with a focus on Schrodinger equation. A review of the Schrodinger equation,

Interpretation, solutions to the non-homogenous Schrodinger equation were among some of the topics which will be treated.

2.1 Review of Schrodinger Equation

Bransden and Co. (2000) stated that, in quantum mechanics, the equation of motion is called the Schrodinger equation. We begin our discussion by considering the one-dimensional, non-relativistic motion of a free particle of mass *m*, having a well-defined momentum $\vec{p} = p_x \hat{x}$ (where \hat{x} is the unit vector along the *x*-axis) of magnitude $p = |p_x|$ and an energy *E*. Assuming that the particle is travelling in the positive *x* direction, then this particle is described by a monochromatic plane wave of wave number $k = \frac{p_x}{h}$ and angular frequency $\omega = \frac{E}{h}$, namely

where A is a constant. The angular frequency ω is connected with the wave number by the relation

$$\omega = \frac{\hbar k^2}{2m}$$
.....2.2a

This equation is equivalent to the classical relation which connects the energy and the momentum of the particle.

Now, by differentiating equation (2.1a) with respect to time, we have

$$\frac{\partial \psi}{\partial t} = -\frac{iE}{\hbar}\psi \dots 2.3a$$

$$\Rightarrow i\hbar \frac{\partial \psi}{\partial t} = E\psi \dots 2.3b$$

On the other hand, differentiating equation (2.1a) twice with respect to x, we have

Substituting (2.5) into (2.4), we have

Equating equations (2.3b) and (2.6), we have

More generally, since equation (2.7) is linear and homogeneous, it will also be satisfied by a linear superposition of plane waves (2.1). For example, the wave packet

associated with a 'localized' free particle moving in one dimension, is also a solution of the equation (2.7), since

The wave Equation (2.7) is known as the *time-dependent Schrodinger equation* for the motion of a *free* particle in *one dimension*.

The generalization of these considerations to free particle motion in 3- dimension is straightforward. The plane wave (2.1b) is given by

It is then readily verified that the plane wave (2.10) satisfies the partial differential equation

is the Laplacian operator.

The wave equation (2.11), which is the direct generalization of equation (2.7), is the three-dimensional time-dependent Schrodinger equation for a free particle. As in the one-dimensional case, it is a linear and homogeneous equation which also satisfies the arbitrary linear superpositions of plane waves (2.10), particularly with the wave packets

$$\psi(\vec{r},t) = \frac{1}{(2\pi\hbar)^{\frac{3}{2}}} \int_{-\infty}^{\infty} dp_x \int_{-\infty}^{\infty} dp_y \int_{-\infty}^{\infty} dp_z e^{\frac{i}{\hbar} [\vec{p},\vec{r}-E(p)t]} \phi(\vec{p}) \dots 2.12a$$

$$=\frac{1}{(2\pi\hbar)^{\frac{3}{2}}}\int e^{\frac{i}{\hbar}[\vec{p}.\vec{r}-E(p)t]}\phi(\vec{p})d\vec{p}$$
2.12b

where $d\vec{p} = dp_x dp_y dp_z$ is the volume element in momentum space.

Equation (2.11) is also clearly of first order in the time derivative $\partial/\partial t$.

Finally, using the fact that in wave mechanics, the total energy E and the momentum p are represented by the differential operators

we observe that the free-particle Schrodinger equation (2.11) may also be written in the form

$$E_{op}\psi(\vec{r},t) = \frac{1}{2m} (p_{op})^2 \psi(\vec{r},t) \dots 2.14$$

in formal analogy with the classical equation (2.2b). We must again note that the

quantity $\vec{p}^2/2m$ is represented by the operator

This equation is called the kinetic energy operator of the particle.

We now want to generalize the free-particle Schrodinger equation (2.11) to the case of a particle moving in a field of force. We shall assume that the force $F(\vec{r},t)$ acting on the particle is derivable from a potential

So that, for a classical particle, the total energy E is given by the sum of its kinetic energy $\vec{p}^2/_{2m}$ and its potential energy $V(\vec{r},t)$

Since the potential energy V does not depend on \vec{p} or E, the above discussion of the free-particle case suggests using equation (2.13) to write

So that the generalization of the free-particle Schrodinger equation (2.11) reads

Equation (2.19) is the celebrated time-dependent Schrodinger wave equation for a particle moving in a potential, which was proposed by E. Schrodinger in 1926. It is the basic equation of non-relativistic quantum mechanics.

The operator appearing inside the brackets on the right of the Schrodinger equation

(2.19) is called the Hamiltonian operator H of the particle. This means that

$$H = -\frac{\hbar^2}{2m} \nabla^2 + V \dots 2.20a$$
$$= -\frac{\hbar^2}{2m} (\vec{p}_{op})^2 + V = T + V \dots 2.20b$$

And the time-dependent Schrodinger equation (2.19) may therefore be rewritten in the form

$$i\hbar \frac{\partial}{\partial t}\psi(\vec{r},t) = H\psi(\vec{r},t)$$
2.21

2.2 Interpretation of Schrodinger equation-Continuity Equation

In reference to equation (2.7), the free particle Schrodinger equation (SE) is given by

$$-\frac{\hbar^2}{2m}\nabla^2\Psi = i\hbar\frac{\partial\Psi}{\partial t}\dots\dots 2.7$$

The complex conjugate equation (SE^*) of (2.7) is

$$-\frac{\hbar^2}{2m}\nabla^2\Psi^* = -i\hbar\frac{\partial\Psi^*}{\partial t}\dots\dots2.22$$

Multiplying equation (2.7) by Ψ^* and (2.22) by Ψ , we have

$$-\frac{\hbar^2}{2m}\Psi^*\nabla^2\Psi = i\hbar\Psi^*\frac{\partial\Psi}{\partial t}\dots 2.23a$$

Subtracting equation (2.23b) from (2.23a), we have

$$-\frac{\hbar^2}{2m}\left(\Psi^*\nabla^2\Psi - \Psi\nabla^2\Psi^*\right) = i\hbar\left(\Psi^*\frac{\partial\Psi}{\partial t} + \Psi\frac{\partial\Psi^*}{\partial t}\right)....2.24a$$

$$\Rightarrow -\frac{\hbar^2}{2m}\vec{\nabla}.\left[\Psi * \vec{\nabla}\Psi - (\vec{\nabla}\Psi *)\Psi\right] = i\hbar \frac{\partial}{\partial t}(\Psi * \Psi)....2.24b$$

By rearranging equation (2.24b) we have

$$\frac{\partial}{\partial t} (\Psi^* \Psi) + \frac{\hbar}{2mi} \vec{\nabla} \cdot \left[\Psi^* \vec{\nabla} \Psi - (\vec{\nabla} \Psi^*) \Psi \right] = 0 \dots 2.25$$

which is just the continuity equation

$$\frac{\partial \rho}{\partial t} + \vec{\nabla}.\vec{j} = 0 \qquad2.26$$

if

$$\vec{j} = \frac{\hbar}{2mi} \Big[\Psi * \vec{\nabla} \Psi - (\vec{\nabla} \Psi *) \Psi \Big] \dots 2.27b$$

Equations (2.27a) and (2.27b) are the probability density and current for the Schrodinger equation.

We now turn to the interpretation of the Klein-Gordon equation. This is nontrivial since the Klein-Gordon equation is of second order in the time derivative

$$\frac{\partial}{\partial t}$$
, which is different from the Schrödinger equation $i\hbar \frac{\partial}{\partial t} \Psi(r,t) = H\Psi(r,t)$,

upon which the probabilistic interpretation of non-relativistic quantum theory is based.

Consider a quantum mechanical problem of scattering of a particle of mass μ and energy *E* by a potential *V*(*r*).

2.3 Solutions to the non-Homogenous Schrodinger wave equation

The Schrodinger wave equation for a particle is given by

where $\Psi(r)$ is the wave function.

Equation (2.28) can be written in the form

$$\left(\nabla^2 - \frac{2\mu}{\hbar^2} V(r)\right) \Psi(r) = -\frac{2\mu}{\hbar^2} E \Psi(r)$$

$$\Rightarrow \left(\nabla^2 + \frac{2\mu E}{\hbar^2}\right)\Psi(r) = \frac{2\mu}{\hbar^2}V(r)\Psi(r) \dots 2.29a$$

Let
$$k^2 = \frac{2\mu E}{\hbar^2}$$
, $U = \frac{2\mu V(r)}{\hbar^2}$

$$\Rightarrow (\nabla^2 + k^2) \Psi(r) = U \Psi(r) \dots 2.29b$$

We then replace the differential equation (2.29b) by an integral equation. The transformation to an integral equation is performed most efficiently by regarding $U\Psi(r)$ on the right-hand side of (2.29) temporarily as a given inhomogeneity, even though it contains the unknown function $\Psi(r)$.

A particular solution of equation (2.29b) is constructed in terms of the Green's function G(r,r') which is the solution of the equation

$$\left(\nabla^2 + k^2\right)G(r, r') = -4\pi\delta(r - r') \dots 2.30$$

Let the expression

$$-\frac{1}{4\pi}\int G(r,r')U(r')\Psi(r')d^{3}r'$$
.....(*)

solves equation (2.30) by virtue of the properties of the delta function and the homogeneous equation

which is the Schrodinger equation for a free particle, that is, no scattering. Solving equation (2.31), we have

$$\Psi(r) = e^{ik.r} \dots 2.32a$$

Choosing a suitable normalization factor, we have equation (2.31) as

$$\Psi(r) = \frac{1}{(2\pi)^{\frac{3}{2}}} e^{ik.r} \dots 2.32b$$

Combining equation (*) and (2.32b), we thus establish the integral equation

$$\Psi(r) = \frac{1}{(2\pi)^{3/2}} e^{i\vec{k}\cdot\vec{r}} - \frac{1}{4\pi} \int G(r,r') U(r') \Psi(r') d^3r' \dots 2.33$$

Equation (2.33) is a particular set of solutions of the Schrodinger equation (2.29b)

 \vec{k} has a definite magnitude, fixed by the energy eigenvalue, but its direction is undetermined thus exhibiting an infinite degree of degeneracy, which corresponds physically to the possibility of choosing an arbitrary direction of incidence.

Even if a particular vector \vec{k} is selected, equation (2.33) is by no means completely defined yet.

The Green's function could be any solution of equation (2.30) and there are infinitely different ones. The choice of a particular $G(\vec{r}, \vec{r}')$ imposes definite boundary conditions on the eigenfunctions $\Psi_k(\vec{r})$.

The two particular useful Green's functions are

A host of Green's function of the form

(

may be obtained by applying a Fourier transformation to the equation

$$\left(\nabla^2 + k^2\right)G(\vec{r}) = -4\pi\delta(\vec{r}) \dots 2.35$$

which is a simplified version of equation (2.30).

We want to introduce

$$G(\vec{r}) = \int g(k')e^{ik'\cdot r} d^3k' \dots 2.36a$$

and the three dimensional delta function defined as

Substituting equations (2.36a) and (2.36b) into (2.35), we have

$$\left(\nabla^2 + k^2 \right) \int g(k') e^{i\vec{k'}\cdot\vec{r}} d^3k' = -4\pi \frac{1}{(2\pi)^3} \int e^{i\vec{k'}\cdot\vec{r}} d^3k' \dots 2.37a$$

$$\Rightarrow \quad \left(\nabla^2 + k^2 \right) g(k') = -\frac{1}{2\pi^2} \dots 2.37b$$

$$\Rightarrow \quad g(k') = -\frac{1}{2\pi^2 \left(\nabla^2 + k^2 \right)} = \frac{1}{2\pi^2 \left(-\nabla^2 - k^2 \right)}$$

$$\left(\nabla^2 + k^2 \right) G(\vec{r}) = -4\pi \frac{1}{(2\pi)^3} \int e^{i\vec{k'}\cdot\vec{r}} d^3k' \dots 2.38a$$

$$\Rightarrow \left(\nabla^2 + k^2 \right) G(\vec{r}) = -\frac{1}{2\pi^2} \int e^{i\vec{k'}\cdot\vec{r}} d^3k' \dots 2.38b$$

$$\Rightarrow \quad G(\vec{r}) = -\frac{1}{2\pi^2} \int \frac{e^{i\vec{k'}\cdot\vec{r}}}{\left(\nabla^2 + k^2 \right)} d^3k' \dots 2.39$$

$$\Rightarrow G(\vec{r}) = \frac{1}{2\pi^2} \int \frac{e^{ik'.r}}{\left(k'^2 - k^2\right)} d^3k' \dots 2.40a$$

and comparing equations (3.9a) and (2.40a), we have

Integrating equation (2.40a) over the solid angles, we have

$$G(\vec{r}) = \frac{1}{2\pi^2} \int_0^{2\pi} d\Psi \int_0^{\pi} \sin\theta d\theta \int_0^{\infty} \frac{e^{ik' \cdot r} k'^2}{k'^2 - k^2} dk' \dots 2.41$$

$$\Rightarrow G(r) = \frac{1}{2\pi^2} 2\pi \int_0^{\pi} e^{ik' \cdot r\cos\theta} \sin\theta d\theta \int_0^{\infty} \frac{k'^2}{k'^2 - k^2} dk' \dots 2.42$$

$$=\frac{1}{\pi}\int_{0}^{\pi}e^{ik'.r\cos\theta}d(-\cos\theta)\int_{0}^{\infty}\frac{k'^{2}}{k'^{2}-k^{2}}dk'$$

$$\Rightarrow G(r) = \frac{1}{ik'\pi r} e^{ik'r\cos\theta} \Big|_0^{\pi} \int_0^{\infty} \frac{k'^2}{k'^2 - k^2} dk'$$

$$\Rightarrow G(r) = \frac{1}{ik'\pi r} \left[e^{-ik'r} - e^{ik'r} \right]_{0}^{\infty} \frac{k'^{2}}{k'^{2} - k^{2}} dk'$$

$$\Rightarrow G(r) = \frac{1}{ik'\pi r} \left[\int_{0}^{\infty} \frac{k'^{2}}{k'^{2} - k^{2}} e^{-ik'r} dk' - \int_{0}^{\infty} \frac{k'^{2}}{k'^{2} - k^{2}} e^{ik'r} dk' \right]$$

$$\Rightarrow G(r) = \frac{i}{\pi r} \left[\int_{0}^{\infty} \frac{k'}{k'^{2} - k^{2}} e^{ik'r} dk' - \int_{0}^{\infty} \frac{k'}{k'^{2} - k^{2}} e^{-ik'r} dk' \right]$$

$$\Rightarrow G(r) = \frac{i}{\pi r} \left[\int_{0}^{\infty} \frac{k'}{k'^{2} - k^{2}} e^{ik'r} dk' + \int_{-\infty}^{0} \frac{k'}{k'^{2} - k^{2}} e^{-ik'r} dk' \right]$$

$$\Rightarrow G(r) = -\frac{1}{\pi r} \left[\frac{d}{dr} \int_{-\infty}^{\infty} \frac{e^{+ikr}}{k'^{2} - k^{2}} dk' \right] \dots 2.43$$

Since the integrand has simple poles on the real axis in the complex k' plane at $k' = \pm k$, the integral (2.43) does not exist, suggesting that our attempt to represent the solutions of (2.30) as Fourier integral has failed. This approach is nevertheless potent because the integral (2.43) can be replaced by another one which does exist. Thus,

$$\Rightarrow G_{+\eta}(r) = -\frac{1}{\pi r} \left[\frac{d}{dr} \int_{-\infty}^{\infty} \frac{e^{+ikr}}{k'^2 - (k^2 + i\eta)} dk' \right] \dots 2.44$$

where η is a small positive number.

 $G_{+\eta}(r)$ exists but is, of course, no longer a solution to equation (2.35). The trick is to evaluate the expression (3.44) for $\eta \neq 0$ and to let $\eta \rightarrow 0$, that is, $G_{+\eta}(r) \rightarrow G_{+}(r)$,

after the positive integration has been performed.

Now, let

$$I = \int_{-\infty}^{\infty} \frac{e^{ik'r}}{k'^2 - (k^2 + i\eta)} dk' \dots 2.45$$

The integral (2.45) is most easily performed by using the complex k'-plane as an auxiliary device.



The path of integration leads along the real axis from $-\infty$ to $+\infty$. A closed contour may be used if we complete the path by a semicircle of very large radius through the upper half plane because r > 0. It encloses the pole in the right half plane. The result of the integration is not changed by introducing detours avoiding the two points

k' = +k and k' = -k. In fact, if this is done, the limit $\eta \to 0$ can be taken prior to the integration and we may write

$$G_{+}(r) = \lim_{\eta \to 0} G_{+\eta}(r) = -\frac{1}{\pi r} \frac{d}{dr} \oint \frac{e^{ik' \cdot r}}{k'^2 - k^2} dk' \dots 2.47$$

According to the residue theorem, we may let f(z) be single-valued and analytic inside and on a simple closed curve C except at the singularities a, b, c, ..., then the residue theorem states that

$$\oint_{C} f(z)dz = 2\pi i (a_{-1} + b_{-1} + c_{-1} + ...) \dots 2.48$$

that is, the integral f(z) around C is $2\pi i$ times the sum of the residues of f(z) at the singularities enclosed by C.

From equation (2.47), if we make use of the residue at k' = +k, then we have

$$G_{+}(r) = -\frac{1}{\pi r} \times 2\pi i \times \frac{d}{dr} \frac{(k'-k)e^{ik'r}}{k'^2 - k^2} \dots 2.49$$

By differentiating equation (2.49) with respect to r, we have

Equation (2.51) is indeed the solution of equation (2.35).

2.4 Positive Energy and Antiparticles of Schrodinger equation

The free particle Schrodinger Equation is given by

which has solution

Substituting equation (2.53) into (2.7) gives

yielding

.2.56b

However, it also has solution

Now, substituting equation (2.55) into (2.7) also gives

E = +

yielding

 ψ_E and ψ_{-E} are different solutions. The first one ψ_E corresponds to positive energy and the second one ψ_{-E} to negative energy. From SE, we have two different solutions for positive and negative energy. This makes it possible to freely toss away one solution as unphysical and keep ψ_E .

Chapter Three

Review of the Relativistic Quantum Mechanics

This chapter also focuses on the review relativistic quantum mechanics. Definition to the relativistic quantum mechanics was unveiled. Other sub-topics which the chapter considered among others were the Minkowski's space, fourvectors, four-velocity, interpretation of Klein-Gordon equation, review of the Dirac equation, positive energy and antiparticles, free particle solutions, and other simple solutions.

3.1.1 Definition of Relativistic Quantum Mechanics

It is the branch of theoretical physics that studies the relativistic (that is, satisfying the requirements of the theory of relativity) quantum laws of motion of micro particles, such as electrons, in what is known as the single-particle approximation. Relativistic effects are great when the energy of a particle is comparable with its rest energy. At such energies, the production of real or virtual particles may occur. For this reason, the single-particle approximation cannot be used in the general case. A consistent description of the properties of relativistic quantum particles is possible only within the framework of quantum field theory. In some problems where relativistic effects are significant, however, particle production need not be taken into consideration, and wave equations describing the motion of one particle of the single-particle approximation can be used. The relativistic corrections to atomic energy levels (fine structure), for example, are found in this way. This approach based on the single-particle approximation is logically unclosed. Thus, in contrast to relativistic quantum

field theory and non-relativistic quantum mechanics, relativistic quantum mechanics, in which problems of this type are considered, does not constitute a consistent theory. Relativistic generalizations of the Schrodinger equation are the basis for calculations in relativistic quantum mechanics: the Dirac equation for electrons and other particles of spin ½ (in units of Planck's constant), and the Klein-Gordon equation for particles of spin 0.

The Klein–Gordon equation (Klein–Fock–Gordon equation or sometimes *Klein–Gordon–Fock equation*) is a relativistic version of the Schrödinger equation.

It is the equation of motion of a quantum scalar or pseudoscalar field, a field whose quanta are spinless particles. It cannot be straightforwardly interpreted as a Schrödinger equation for a quantum state, because it is second order in time and because it does not admit a positive definite conserved probability density. Still, with the appropriate interpretation, it does describe the quantum amplitude for finding a point particle in various places, the relativistic wavefunction, but the particle propagates both forwards and backwards in time. Any solution to the Dirac equation is automatically a solution to the Klein–Gordon equation, but the converse is not true.

3.1.2 Minkowski's Space

Minkowski pointed out that the external world is not formed of ordinary three dimensional space, known as Euclidean space, but it is four dimensional space-time continuum known as Minkowski or World space, where time or more conveniently *ict* may be regarded to be the fourth dimension. Therefore, an event in world space must be represented by four coordinates (x_1, x_2, x_3, x_4) out of which the first three

are space coordinates and the fourth one is the time coordinate. The events in the world are represented by points known as world points. In this world space, there corresponds to each particle a certain line known as world line. Let us consider two axes *OX* and *OP*. O being the origin of the system (where p = ict).

According to Lorentz transformations,

$$x^{2} + y^{2} + z^{2} - c^{2}t^{2} =$$
 invariant.
 $y' = y, z' = z$.

But

$$\Rightarrow x^2 - c^2 t^2 = x^2 + p^2 = \text{invariant.}$$

This means that the distance of any variable point P in x-p plane from origin is unchanged.

3.1.3 Four-vectors

Having introduced the idea of four-dimensional space, it is possible to extend ordinary vector analysis to four dimensions to derive generally valid laws in the form of equations between four dimensional vector. These four dimensional vectors are called four vectors or world vectors.

A four-vector in the x_1 , x_2 , x_3 , x_4 space is defined as a quantity which transformations under Lorentz transformation in the same way as the x_1 , x_2 , x_3 , x_4 co-ordinates of a point in the four dimensional space. It must be noted that the length of a 4-vector is unchanged under Lorentz transformation. If the square of the length of a 4-vector is positive, it is space-like vector and if the 4-vector is negative, it is also time-like vector. The position of the component of a 4-vector is represented by

$$A_{\mu} = (A_1, A_2, A_3, A_4) = (A, iA_0)$$

The square of the magnitude of the vector

$$A_{\mu}A_{\mu} = A_1^2 + A_2^2 + A_3^2 - A_0^2$$

3.1.4 4-Velocity

A 4-velocity vector u_{v} is defined by

Κ	$u_v = \frac{dx_v}{d\tau}$

where $x_v = (x, ict)$ and $d\tau$ is the proper time given by



3.1.5 Relationship between proper time and an ordinary time

If the form of a law is not changed by certain coordinate transformation, the law is said to be invariant. If any physical law may be expressed in a covariant four dimensional form, then the law will be invariant under *Lorentz transformations*. In four dimensions, the position vector will be termed as position four-vector. The position four-vector in four dimensions will be represented as

$$\underline{r} = \hat{x}_1 x_1 + \hat{x}_2 x_2 + \hat{x}_3 x_3 + \hat{x}_4 x_4$$

where \hat{x}_1 , \hat{x}_2 , \hat{x}_3 and \hat{x}_4 are unit vectors along x_1 , x_2 , x_3 and x_4 respectively. To differentiate position four-vector with ordinary position vector, we have to put <u>r</u> in place of r.

Taking dot product of \underline{r} with itself, we shall get a world scalar and hence *Lorentz invariant*, that is,

$$\underline{r} \cdot \underline{r} = (\hat{x}_1 x_1 + \hat{x}_2 x_2 + \hat{x}_3 x_3 + \hat{x}_4 x_4) (\hat{x}_1 x_1 + \hat{x}_2 x_2 + \hat{x}_3 x_3 + \hat{x}_4 x_4)$$

$$\Rightarrow \underline{r} \cdot \underline{r} = x_1^2 + x_2^2 + x_3^2 + x_4^2 = \text{Lorentz invariant.}$$

If $d\underline{r}$ represents the change in position four vector, then we have

$$d\underline{r} = \hat{x}_1 dx_1 + \hat{x}_2 dx_2 + \hat{x}_3 dx_3 + \hat{x}_4 dx_4$$

Taking dot product of this with itself, we shall get a world scalar and hence

Lorentz invariant, that is,

$$\underline{dr} \cdot \underline{dr} = (\hat{x}_1 dx_1 + \hat{x}_2 dx_2 + \hat{x}_3 dx_3 + \hat{x}_4 dx_4)(\hat{x}_1 dx_1 + \hat{x}_2 dx_2 + \hat{x}_3 dx_3 + \hat{x}_4 dx_4)$$

$$\Rightarrow \underline{dr} \cdot \underline{dr} = dx_1^2 + dx_2^2 + dx_3^2 + dx_4^2 = \text{Lorentz invariant}$$
or
$$\underline{dr}^2 = dx_1^2 + dx_2^2 + dx_3^2 + dx_4^2$$
But
$$x_1 = x, x_2 = y, x_3 = z \text{ and } x_4 = ict$$

$$\therefore \underline{dr} \cdot \underline{dr} = \underline{dr}^2 = dx^2 + dy^2 + dz^2 - c^2 dt^2 = \text{Lorentz invariant.}$$

If we consider a system in which a particle is momentarily at rest, as the object is at rest, its displacement vanishes, that is, dx = 0, dy = 0, dz = 0 and let the time be denoted by τ , then we have

As dr^2 is an invariant, we have

$$\underline{dr}^{2} = dx^{2} + dy^{2} + dz^{2} - c^{2}dt^{2} = -c^{2}d\tau^{2}$$
....(b)

From equation (a), it is clear that $d\tau = -\frac{dr}{ic}$ is an invariant, dr and c are also invariant.

The time $d\tau$, as measured in the rest frame is called the proper time.

A proper time is a time measured by the clock fixed in the rest frame of the particle. It is a scalar or invariant under Lorentz transformation.

From equation (b), we have

$$d\tau^{2} = dt^{2} - \frac{1}{c^{2}} \left(dx^{2} + dy^{2} + dz^{2} \right)$$
$$\Rightarrow d\tau^{2} = dt^{2} \left[1 - \frac{1}{c^{2}} \left(\left(\frac{dx}{dt} \right)^{2} + \left(\frac{dy}{dt} \right)^{2} + \left(\frac{dz}{dt} \right)^{2} \right) \right]$$
$$d\tau = dt \sqrt{1 - \frac{v^{2}}{c^{2}}} \qquad \Rightarrow d\tau = dt \sqrt{1 - \beta^{2}}$$

This is an expression for time dilation.

where

3.2 Review of the Hamiltonian and the Klein-Gordon Equation

 $\beta = \frac{v}{c}$.

Let the dynamical properties of a classical particle of rest mass be 'm' and 'e' in an electromagnetic field and let 'v' be the velocity of the particle. In Newtonian presentation, the velocity vector 'v' is given by

From the equation

 $\frac{d\tau}{dt} = \sqrt{1 - \beta^2}$

We define the relativistic mass M and the Mechanical momentum p by
$$M = \frac{m}{\sqrt{1 - \vec{v}^{2}}} \quad and \quad M\vec{v} = \frac{m\vec{v}}{\sqrt{1 - \vec{v}^{2}}} \dots 3.2$$
$$\vec{P} = \frac{m\vec{v}}{\sqrt{1 - \vec{v}^{2}}} \dots 3.3$$

where

 $\vec{P} = M\vec{v}$

Equation (3.3) forms a certain four -vector

That is,

and pointing into the future, E > 0

In the absence of a field, the particle follows a uniform rectilinear motion with v = constant

According to Jackson(1962), in the electromagnetic field, the trajectory followed by the particle satisfies the equation

$$\frac{d\vec{p}}{dt} = q(\vec{E} + \vec{v} \times \vec{H}) = \vec{F} \dots 3.5$$

This is the fundamental equation of the relativistic dynamics of a material point.

The vector \vec{F} is called the Lorentz force.

The relativistic velocity u_v is defined as

$$\Rightarrow p_{v} = \left(\vec{p}, \frac{i}{c}E\right).....3.8$$

where

$$E = \frac{mc^2}{\sqrt{1-\beta^2}}$$
 and $\vec{p} = \frac{m\vec{v}}{\sqrt{1-\beta^2}}$

 p_{v} is called the 4-vector momentum and \vec{p} is also the 3-dimensional momentum. Using the condition that the length of a 4-vector is invariant,

$$p_{\nu}p_{\nu} = p^2 - \frac{E^2}{c^2} = \text{constant} \dots 3.9$$

When

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$$\Rightarrow p^2 - \frac{E^2}{c^2} = -m^2 c^2 \dots 2.32$$

$$\Rightarrow E^2 = c^2 p^2 + m^2 c^4 \dots 3.11a$$

In a magnetic field, the velocity v is given by

$$V = -q\Phi + \frac{q}{c}\vec{A}.\vec{V} \qquad3.12$$

where Φ is a scalar potential.

A system is said to be conserved if its energy is constant. In such a system, the

Hamiltonian

where T is the kinetic energy and V is the potential energy.

In a non-relativistic case,

$$T = \frac{1}{2}mV^2 \dots 3.14$$

The Lagrangian L is also given by

$$L = \frac{1}{2}mV^{2} - q\phi + \frac{q}{c}\vec{A}.\vec{V} \dots 3.15$$

By differentiating with respect to V,

$$\Rightarrow \quad \vec{p}_L = \frac{dL}{dV} = m\vec{V} + \frac{q}{c}\vec{A} \dots 3.16a$$

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By making \vec{V} the subject,

$$\Rightarrow \quad \vec{V} = \frac{1}{m} \left(\vec{p}_L - \frac{q}{c} \vec{A} \right) \dots 3.16b$$

By squaring both sides of equation (3.16b),

.

$$\Rightarrow V^2 = \vec{V}.\vec{V} = \frac{1}{m^2} \left(\vec{p}_L - \frac{q}{c} \vec{A} \right)^2 \dots 3.17$$

Multiplying through equation (3.17) by m^2

$$\Rightarrow m^2 V^2 = \left(\vec{p}_L - \frac{q}{c}\vec{A}\right)^2 \dots 3.18a$$

$$\Rightarrow p^2 = \left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 \dots 3.18b$$

Substituting equation (3.11b) into (3.13),

$$\Rightarrow H = \sqrt{c^2 p^2 + m^2 c^4} + \vec{V} \dots 3.19$$

Substituting equation (3.18b) into equation (3.19),

$$\Rightarrow H = \sqrt{c^2 \left(\vec{p} - \frac{q}{c}\vec{A}\right)^2 + m^2 c^4} + q\Phi \dots 3.20$$

where $V = q\Phi$

Equation (3.20) is the relativistic expression for a particle in an electromagnetic field

Now since the problem of finding a relativistic wave equation for the electron is complicated by the existence of spin, we first look for a relativistic wave equation for a particle of spin 0. Such a particle has no internal degrees of freedom and so its wave function Ψ depends only on the variables \vec{r} and t.

Let 'm' be the mass of such a particle and 'q' its charge. Suppose that it is moving in the electromagnetic potential

$$A^{\mu} = (\Phi, \overline{A}) \dots 3.21$$

To find the wave equation, we proceed empirically using the correspondence principle and this will guarantee that we can obtain the classical laws of motion when the classical approximation is valid. The Schrödinger correspondence rule is given by:

From $P^{\mu} = (E, \vec{p})$ and the Hamiltonian equation (3.20),

$$H = \vec{E} = q\Phi + \sqrt{\left(\vec{p} - q\vec{A}\right)^2 + m^2 c^4} \dots 3.23$$

Substituting equation (3.22) into (3.23),

$$\Rightarrow i\hbar \frac{\partial}{\partial t} = q\Phi + \sqrt{\left(-i\hbar\nabla - q\vec{A}\right)^2 + m^2 c^4} \dots 3.24a$$

Multiplying both sides of equation (3.24a) by wave function Ψ

$$\Rightarrow (i\hbar\frac{\partial}{\partial t} - q\Phi)\Psi = \left[\left(\frac{i}{\hbar}\nabla - q\vec{A}\right)^2 + m^2c^4\right]^{\frac{1}{2}}\Psi \dots 3.24b$$

Equation (3.24b) has two main drawbacks

First, the dissymmetry between the space and time coordinates is such that

relativistic invariance and its consequences are not clearly exhibited.

Secondly, the operator on the right hand side is a square root which is practically unatractable except when the field \vec{A} vanishes.

Now to avoid these two difficulties, we take equation (3.4) as the starting point of the correspondence operation and the fact that

Substituting (3.25) into (3.4), we have

Equation (3.26) is equivalent to the more general equation

It must be noted that

(i) Only the positive sign corresponds to real classical solutions

(ii) The negative sign represents solutions of negative energy without any physical significance.

By taking equation (3.26) as the starting point and applying the correspondence operation and the wave function, we have

Expanding the LHS of equation (3.28), we have

$$\left[\left(-\hbar^2\frac{\partial^2}{\partial t^2}-i\hbar q\frac{\partial\Phi}{\partial t}-i\hbar q\Phi\frac{\partial}{\partial t}+q^2\Phi^2\right)-\left(-\hbar^2\nabla^2+i\hbar q\nabla.\vec{A}+i\hbar qA.\nabla+q^2\vec{A}^2\right)\right]\Psi=m^2c^4\Psi\ldots 3.29$$

By re-arranging the terms, we have

$$\left[-\hbar^2(\frac{\partial^2}{\partial t^2}-\nabla^2)+q^2(\Phi^2-\vec{A}^2)-i\hbar q(\nabla.\vec{A}+\frac{\partial\Phi}{\partial t})-i\hbar q(\Phi\frac{\partial}{\partial t}+\vec{A}.\nabla)\right]\Psi=m^2c^4\Psi\dots 3.30$$

In a weak field,

$$q^2(\Phi^2 - \vec{A}^2) = 0$$
 and by Lorentz gauge,

Equation (3.30) will reduce to

$$\left[-\hbar^2 (\frac{\partial^2}{\partial t^2} - \nabla^2) - i\hbar q (\Phi \frac{\partial}{\partial t} + \vec{A} \cdot \nabla)\right] \Psi = m^2 c^4 \Psi \dots 3.32a$$

$$\Rightarrow \left[\hbar^{2} \left(\frac{\partial^{2}}{\partial t^{2}} - c^{2} \nabla^{2}\right) + m^{2} c^{4}\right] \Psi = i\hbar q (\vec{A} \cdot \nabla + \Phi \frac{\partial}{\partial t}) \Psi \dots 3.32b$$

$$(\Box^{2} + m^{2}c^{4})\Psi = i\hbar q(\vec{A}.\nabla + \Phi\frac{\partial}{\partial t})\Psi \dots 3.33$$

where

Equation (3.34) is commonly referred to as D'Alembertian operator

Now from equation (3.33), if we consider a free particle of spin 0, then we have

If we substitute equation (3.34) into (3.35), we have

$$\left[\hbar^2 \left(\frac{\partial^2}{\partial t^2} - c^2 \nabla^2\right) + m^2 c^4\right] \Psi = 0 \dots 3.36a$$

$$\Rightarrow -\hbar^2 \frac{\partial^2 \Psi}{\partial t^2} + \hbar^2 c^2 \nabla^2 \Psi - m^2 c^4 \Psi = 0 \dots 3.36b$$

$$\Rightarrow -\hbar^2 \frac{\partial^2 \Psi}{\partial t^2} = m^2 c^4 \Psi - \hbar^2 c^2 \nabla^2 \Psi \dots 3.36c$$

Equation (3.35) is the homogenous Klein-Gordon Equation for a free particle.

3.3 Interpretation of Klein-Gordon Equations: Continuity Equation

The Klein-Gordon equation was historically rejected because it predicted a negative probability density. In order to see this, let us first revise the probability and current for the Schrodinger equation.

In order to simplify the discussion, we shall consider only the free particle Klein-Gordon equation

$$-\hbar^2 \frac{\partial^2}{\partial t^2} \Psi = m^2 c^4 \Psi - \hbar^2 c^2 \nabla^2 \Psi \dots 3.36c$$

To interpret the wave function, let us try to construct a position probability density P(r,t) and a probability current density j(r,t) satisfying the continuity equation

$$\frac{\partial \rho}{\partial t} + \nabla . j = 0 \dots 3.37$$

If Ψ is a solution to the Klein-Gordon equation (3.36c), then its complex conjugate Ψ^* must also be a solution to the Klein-Gordon equation. This means that we can write the complex conjugate of equation (3.36c) as

Multiplying through equation (3.36c) by Ψ^* on the Left Hand Side, equation (3.38) by Ψ on the Right Hand Side, we have

And subtracting these equations, we also have

$$\Psi^* \frac{\partial^2 \Psi}{\partial t^2} - \Psi \frac{\partial^2 \Psi^*}{\partial t^2} = c^2 \left[\Psi^* \nabla^2 \Psi - \Psi \nabla^2 \Psi^* \right] \dots 3.40a$$
$$\frac{\partial}{\partial t} \left(\Psi^* \frac{\partial \Psi}{\partial t} - \Psi \frac{\partial \Psi^*}{\partial t} \right) = \vec{\nabla} \cdot \left[\Psi^* \vec{\nabla} \Psi - \Psi \nabla^2 \Psi^* \right] \dots 3.40b$$
which is the continuity equation
$$\frac{\partial \rho}{\partial t} + \vec{\nabla} \cdot \vec{j} = 0 \dots 3.37$$

If

then
$$\vec{j} = \Psi \vec{\nabla} \Psi^* - \Psi^* \vec{\nabla} \Psi$$
 or $j^{\mu} = \Psi^* \partial^{\mu} \Psi - \Psi \partial^{\mu} \Psi^{\mu} \dots 3.41b$

But for this equation to match the Schrodinger Equation wave function, we

should define \vec{j} in the same way, i.e.

$$\vec{j} = \frac{\hbar}{2mi} \left[\Psi * \vec{\nabla} \Psi - \Psi \vec{\nabla} \Psi^* \right] = \frac{-i\hbar}{2m} \left(\Psi^* \vec{\nabla} \Psi - \Psi \nabla \Psi^* \right) \dots 3.42$$

Thus for equation (2.60) to hold, we must have

$$\rho = \frac{i\hbar}{2m} \left(\Psi^* \frac{\partial \Psi}{\partial t} - \Psi \frac{\partial \Psi^*}{\partial t} \right) \dots 3.43$$

The problem with ρ (in both expressions above) is that it is not positive definite and therefore cannot be interpreted as a probability density. This is one reason why Klein-Gordon equation was discarded.

According to Landau (1977), because ρ can be either positive or negative, it can be interpreted as charge density. We therefore note that this problematic

 ρ came about because the Klein-Gordon equation is a 2nd order in time. We have $\frac{\partial \rho}{\partial t}$ and ρ itself constrains $\frac{\partial}{\partial t}$; this does not happen with the Schrodinger equation

and Dirac equation.

3.4 Fourier expansion and momentum space

As with the non-relativistic case, we expand plane wave states as

$$\Psi(\vec{r},t) = \int d\vec{k} \,\phi(\vec{k},t) e^{ik.\vec{r}} \dots 3.44$$

But now with

$$d\tilde{k} = N_k d^3 k \dots 3.45a$$

where N_k is a normalization constant which is given by

$$N_k = \frac{1}{2\omega(2\pi)^3} \dots 3.45b$$

Substituting $\Psi(\vec{r},t)$ into the free Klein-Gordon equation

$$\Rightarrow -\hbar^2 \frac{\partial^2 \Psi}{\partial t^2} + \hbar^2 \nabla^2 \Psi - m^2 \Psi = 0$$

This gives us

$$\int d\tilde{k} \left(\ddot{\phi} + k^2 \phi + m^2 \phi \right) e^{ik.\bar{r}} = 0 \dots 3.46$$

Now, defining

$$\omega \equiv \omega(\vec{k}) = \sqrt{k^2 + m^2} \quad \dots \quad 3.47$$

and requiring the integrand to be zero gives

$$\phi + \omega^2 \phi = 0 \dots 3.48$$

which is a 2nd order differential equation, with auxiliary equation

$$r^2 + \omega^2 = 0 \quad or \quad r = \pm i\omega \dots 3.49$$

The two solutions are crucial! They can be interpreted as positive and negative energy, or as particle and antiparticle. In the non-relativistic case, we only have one solution

$$\phi(\vec{k},t) = a(\vec{k})e^{i\omega t} + c(\vec{k})e^{-i\omega t} \dots 3.50$$

3.5 Review of Dirac Equation

From Zaarur and Co. (1998), spin is an intrinsic property of particles. The definition of spin operator S is analogous to the angular momentum operator

 $|\alpha\rangle$ being an eigenfunction of S^2 and S(S+1) the corresponding eigenvalues.

We can also define

where S_x, S_y and S_z obey the following commutation relations:

Analogous to angular momentum, the quantum number of spin in the z-direction

is

$$m_s = -S, -S + 1, \dots, +S$$
 and

For particles (an electron, for example) with spin $\frac{1}{2}$, we have $m_s = \pm \frac{1}{2}$ and two distinct eigenvectors of S^2 and S_z denoted by $\left|+\frac{1}{2}\right\rangle$ and $\left|-\frac{1}{2}\right\rangle$. These

eigenvectors are called the standard basis, where

$$S^{2}\left|\pm\frac{1}{2}\right\rangle = \frac{3}{4}\hbar^{2}\left|\pm\frac{1}{2}\right\rangle, \qquad S_{z}\left|\pm\frac{1}{2}\right\rangle = \pm\frac{\hbar}{2}\left|\pm\frac{1}{2}\right\rangle.$$

$$(3.55)$$

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The Pauli matrices $\sigma = (\sigma_x, \sigma_y, \sigma_z)$ are defined using

$$S = \frac{\hbar}{2}\sigma \dots 3.56$$

where

$$\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
....3.57

S being written in the standard basis. The commutation relations of the Pauli matrices are

$$[\sigma_x, \sigma_y] = 2i\sigma_z, \ [\sigma_y, \sigma_z] = 2i\sigma_x, \ [\sigma_z, \sigma_x] = 2i\sigma_y.....3.58$$

Other useful relations of Pauli matrices are

$$\sigma_x^2 = \sigma_y^2 = \sigma_z^2 = 1.....3.59$$

Consider a system consisting of particles with a spin S. Applying a magnetic field B will introduce an additional term to the free Hamiltonian H_0 , so that

$$H = H_0 + H_{int} = H_0 + \frac{eB}{mc} \cdot S \dots 3.60$$

Hence the electron spin magnetic moment or interaction H_{int} is

$$H_{\rm int} = -\left(\frac{eB}{mc}\right) \cdot \frac{\hbar}{2}\sigma = -\left(\frac{e\hbar}{2mc}\right)\sigma \cdot B \dots 3.61$$

We have already seen that the Klein Gordon Equation gives rise to negative energies and non-positive definite probabilities and these reasons were discarded as a fundamental quantum equation. These problems arise because the Klein-Gordon equation is non-linear in $\frac{\partial}{\partial t}$, unlike the Schrodinger Equation. Dirac thus sought a relativistic quantum equation linear in $\frac{\partial}{\partial t}$, unlike the Schrodinger Equation. Dirac therefore invented a matrix equation.

Sakurai (1967) also stated that Klein-Gordon equation could not accommodate

the $Spin - \frac{1}{2}$ nature as the Dirac equation can. In this connection, let us first study how to incorporate the electron spin in the non-relativistic quantum mechanics.

In non-relativistic quantum mechanics, in order to account for the interaction of the electron spin magnetic moment with the magnetic field, it is customary to add a term

$$H^{(spin)} = -(e\hbar/2mc)\sigma.\vec{B} \dots 3.62$$

to the usual Hamiltonian, as done originally by W.Pauli. Consider a particle of mass m and charge e moving in an electromagnetic field described by a vector potential $A(\vec{r},t)$ and a scalar potential $A_0(\vec{r},t)$. Its non-relativistic classical Hamiltonian can be obtained by starting from the particle, and making in it the substitutions

This procedure appears somewhat artificial, especially if we subscribe to the philosophy that the only fundamental electromagnetic interactions are those which can be generated by the substitution

In the usual wave mechanical treatment of the electron, the kinetic energy

operator in the absence of the vector potential is given by

However, for a $Spin - \frac{1}{2}$ particle, we may just as well start with the expression

$$H^{(K.E)} = (\sigma.\vec{p})(\sigma.\vec{p})/2m\dots 3.66$$

This alternative form is indistinguishable from equation (3.65) for all practical purposes when there is no vector potential. There is, however, a difference when we make the substitution of equation (3.64).

The expression (3.65) then becomes

and the formula

$$(\sigma.\vec{A})(\sigma.\vec{B}) = \vec{A}.\vec{B} + i\sigma.(\vec{A} \times \vec{B}) \dots 3.68b$$

holds even if A and B are operators.

Our objective is to derive a relativistic wave equation for $Spin - \frac{1}{2}$ particle. Just as we incorporated the electron spin into the general framework of relativistic theory using the kinetic energy operator (3.66), we can in the same way incorporate the electron spin into the general framework of relativistic quantum mechanics by taken the operator analog of the classical expression

$$\left(\frac{E^{(op)}}{c} - \sigma.\vec{p}\right) \left(\frac{E^{(op)}}{c} + \sigma.\vec{p}\right) = (mc)^2 \dots (3.69b)$$

where

$$E^{(op)} = i\hbar \frac{\partial}{\partial t} = i\hbar \frac{\partial}{\partial x_0} \text{ and } \vec{p} = -i\hbar \nabla.....2.13$$

This enables us to write a second-order equation

$$\left(i\hbar\frac{\partial}{\partial x_0} + \sigma .i\hbar\nabla\right)\left(i\hbar\frac{\partial}{\partial x_0} - \sigma .i\hbar\nabla\right)\Phi = (mc)^2\Phi \dots 3.70$$

for a free electron, where Φ is now a *two-component* wave function.

We are interested in obtaining a wave equation of first order in the time derivative. Relativistic covariance suggests that the wave equation linear in $\partial/\partial t$ must be linear in ∇ also.

We can therefore define *two-component* wave functions $\Phi^{(R)}$ and $\Phi^{(L)}$ where

$$\Phi^{(R)} = \frac{1}{mc} \left(i\hbar \frac{\partial}{\partial x_0} - i\hbar\sigma . \nabla \right) \Phi, \quad \Phi^{(L)} = \Phi \dots 3.71 a$$

From equation (3.70), it implies that

$$\left(i\hbar\frac{\partial}{\partial x_0} + \sigma.i\hbar\nabla\right)\Phi^{(R)} = mc\Phi^{(L)} \dots 3.71b$$

The total number of components has now been increased to four. The secondorder equation (3.70) is now equivalent to two first-order equations (3.72a) and (3.72b)

Equation (3.72) is equivalent to the wave equation of Dirac. To bring it to form originally written by Dirac, we take the sum and difference of equation (3.72).

We then have

Denoting the sum and difference of $\Phi^{(R)}$ and $\Phi^{(L)}$ by Ψ_A and Ψ_B , we have

Defining a four component wave function Ψ by

$$\Psi = \begin{pmatrix} \Psi_A \\ \Psi_B \end{pmatrix} = \begin{pmatrix} \Phi^{(R)} + \Phi^{(L)} \\ \Phi^{(R)} - \Phi^{(L)} \end{pmatrix} \dots 3.75$$

We can rewrite (3.74) more concise as

$$\left(\gamma \cdot \nabla + \gamma_4 \frac{\partial}{\partial (ix_0)}\right) \Psi + \frac{mc}{\hbar} \Psi = 0 \dots 3.76a$$

or
$$\left(\gamma_\mu \frac{\partial}{\partial x_\mu} + \frac{mc}{\hbar}\right) \Psi = 0 \dots 3.76b$$

where γ_{μ} with $\mu = 1, 2, 3, 4$ are 4×4 matrices given by

$$\gamma_{k} = \begin{pmatrix} 0 & -i\sigma_{k} \\ i\sigma_{k} & 0 \end{pmatrix}, \qquad \gamma_{4} = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}.....3.77$$

Which really mean

$$\gamma_{3} = \begin{pmatrix} 0 & 0 & -i & 0 \\ 0 & 0 & 0 & i \\ i & 0 & 0 & 0 \\ 0 & -i & 0 & 0 \end{pmatrix}, \qquad \gamma_{4} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad etc. \dots ...3.78$$

It must be noted that the standard form of the Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$
....3.79

were used.

The symbol I also stand for the 2×2 identity matrix

Multiplying equation (3.76a) by γ_4 , we see that the Dirac equation can be written in the Hamiltonian form

$$H\Psi = i\hbar \left(\frac{\partial\Psi}{\partial t}\right)......3.81$$

$$H = -ic\hbar\alpha \cdot \nabla + \beta mc^2 \dots 3.82$$

where

$$\Rightarrow i\hbar \frac{\partial \Psi}{\partial t} = -i\hbar\sigma . \nabla \Psi + \beta mc^2 \Psi \dots 3.83$$

with

$$\beta = \gamma_4 = \begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix}, \qquad \alpha_k = i\gamma_4\gamma_k = \begin{pmatrix} 0 & \sigma_k \\ \sigma_k & 0 \end{pmatrix}.....3.84$$

The matrices α and β satisfy

3.6 Probability and current for Dirac Equation

According to Norbury (2000), for the Schrodinger Equation(SE) and Klein-Gordon equation(KGE), we used Schrodinger equation (SE*) Klein-Gordon equation (KGE*) to derive the continuity equation. For matrices, the generalization of the complex conjugate (*) is Hermitian conjugate (+) which is the transpose of the complex conjugate. The Dirac equation is

$$(i\partial - m)\psi = 0.....3.86a$$

$$\Rightarrow \left(i\gamma^{\mu}\partial_{\mu}-m\right)=0.....3.86b$$

and $DE^* = DE^+$ is (using $(AB)^+ = B^+A^+$) given by

where

making using of

$$\gamma^{\mu+} = \gamma^{\mu}\gamma^{\mu}\gamma^{0} \dots 3.91$$

We want to introduce the Dirac adjoint (ψ is a column matrix)

Using $\gamma^0 \gamma^0 = 1$, we get

$$\psi^{+}(-i\gamma^{0}\gamma^{\mu}\gamma^{0}\partial_{\mu}-m\gamma^{0}\gamma^{0})=0.....3.93$$

$$\Rightarrow \overline{\psi} (i \gamma^{\mu} \gamma^{0} \partial_{\mu} + m \gamma^{0}) = 0 \dots 3.94$$

And cancelling out γ^0 gives, the Dirac adjoint equation,

The notation $\overline{\partial}$ means that ∂ operates on $\overline{\psi}$ to the left, i.e. $\overline{\psi} \overline{\partial} \equiv (\partial_{\mu} \overline{\psi}) \gamma^{\mu}$.

The DE and DE^+ are explicitly

Now, to derive the continuity equation, multiply Differential Equation (DE)

from the left by $\overline{\psi}$ and DE^+ from the right by ψ , we have

and

$$\overline{\psi}(i\gamma^{\mu}\partial_{\mu}\psi - m\psi) = 0.....3.97a$$

$$\left(i(\partial_{\mu}\overline{\psi})\gamma^{\mu} + m\overline{\psi}\right)\psi = 0.....3.97b$$

Adding these two equations, we have

$$\overline{\psi}\gamma^{\mu}\partial_{\mu}\psi + (\partial_{\mu}\overline{\psi})\gamma^{\mu}\psi = 0 = \partial_{\mu}(\overline{\psi}\gamma^{\mu}\psi) \dots 3.98$$

NO

Giving

$$j^{\mu} = (\overline{\psi}\gamma^{\mu}\psi) \equiv (\rho, \overline{j}) \dots 3.99$$

which is now positive definite.

3.7 Positive Energy and Antiparticles

For the cases in Klein-Gordon equation and Differential Equation, we always have both positive and negative for all solutions. The only way to toss away the negative energy is to toss away all solutions; i.e. toss out the whole equation.

3.7.1 Klein Gordon equation

From the free particle Klein Gordon Equation which is given by

$$\Rightarrow -\hbar^2 \frac{\partial^2 \Psi}{\partial t^2} + \hbar^2 \nabla^2 \Psi - m^2 \Psi = 0 \dots 3.36c$$

1.1

be a solution.

Substituting (3.101) into (3.36c) gives

which implies

Thus the single solution $\phi = Ne^{ip.x} = N^{i(Et-\overline{p}.\overline{x})}$ has both positive and negative energy

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solutions.

Another solution is $\phi = Ne^{-ip.x}$.

Substituting also into the free KGE give the same as above

$$(E^2 - \vec{p}^2 + m^2)\phi = 0$$
.....3.104a

And again, a single solution $\phi = Ne^{-ip.x}$ has both positive and negative energy solutions.

The interpretation of these states is as follows. For $\vec{p} = 0$ (particle at rest), then $E = \pm m$. For $\vec{p} \neq 0$, there will be a continuum of states above and below $E = \pm m$, with bound states appearing in between. In quantum mechanics, there will be transitions to the negative energy continuum to infinite negative energy. The Klein-Gordon equation then becomes a relativistic wave equation for spinless particles, within the framework of *many-particle* theory in which the negative energy states are interpreted in terms of *antiparticles*.

3.7.2 Dirac equation

Let us return to the Dirac equation (3.83) for a free particle of $Spin - \frac{1}{2}$. Since the Hamiltonian (3.82) is independent of *r* and *t*, we can seek the eigenfunctions common to both the energy and momentum operators, namely plane waves of the form

where A is a constant and u is a four-component spinor independent of x and t. The plane waves (3.105) are eigenfunctions of the operators

 $E = i\hbar \frac{\partial}{\partial t}$ and $P = -i\hbar \nabla$ with eigenvalues $E = \hbar \omega$ and $p = \hbar k$, respectively.

Substituting equation (3.105) into (3.83) gives for u the matrix equation.

For a *particle at rest* $p \approx 0$, equation (3.105a) becomes

$$\left(\beta mc^2\right)u = Eu \dots 3.105b$$

Denoting the corresponding four-component spinor by $u(0) = \begin{pmatrix} u_A(0) \\ u_B(0) \end{pmatrix}$ and in

accordance with equations (3.75) and (3.76), we first try the time-

dependence $e^{-imc^2t/\hbar}$. Using equation (3.84), equation (3.105b) then reduces to

$$\begin{pmatrix} I & 0 \\ 0 & -I \end{pmatrix} mc^{2} u(0) = Eu(0) \dots 3.106a$$
$$\Rightarrow \begin{pmatrix} mc^{2}I & 0 \\ 0 & -mc^{2}I \end{pmatrix} u(0) = Eu(0) \dots 3.106b$$
$$\Rightarrow \begin{pmatrix} mc^{2}I & 0 \\ 0 & -mc^{2}I \end{pmatrix} \begin{pmatrix} u_{A}(0) \\ u_{B}(0) \end{pmatrix} = E \begin{pmatrix} u_{A}(0) \\ u_{B}(0) \end{pmatrix} \dots 3.106c$$

Equation (3.106c) is satisfied only if the lower two-component spinor

 $u_B(0)$ vanishes. But using a similar argument, we also see that equation (3.105) can be satisfied equally well by the time-dependence $e^{+imc^2t/\hbar}$ provided that the upper two-component spinor $u_A(0)$ vanishes.

As in the Pauli theory, the non-vanishing two-component spinors can be taken as

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} and \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

So there are four independent solutions to equation (3.105b):



two are "positive-energy" solutions while the last two are "negative –energy" solutions. It must also be note that the eigenvalues of the Hamiltonian operator , depending on whether the eigenvalues of $\gamma_4 = \beta$ are ± 1 . are $\pm mc^2$

3.8 Free particle solution

Let us now consider the case $p \neq 0$. It is convenient to write the four-component spinor u in terms of two-component spinors $u_A(p)$ and $u_B(p)$ as

From equation (3.105a),

and making use of equation (3.109), we can have

$$\begin{pmatrix} mc^2 I & c\sigma.p \\ c\sigma.p & -mc^2 I \end{pmatrix} u(p) = Eu(p).....3.110a$$

From equation (3.110b)

$$\Rightarrow mc^{2}Iu_{A} + c\sigma.pu_{B} = Eu_{A}.....3.111a$$

and
$$c\sigma.pu_{A} - mc^{2}Iu_{B} = Eu_{B}.....3.111k$$

Modifying equation (3.111), we have

 $u_A(p)$ and $u_B(p)$ are now related according to (3.112) by

$$u_{A}(p) = \frac{c\sigma.p}{E - mc^{2}} u_{B}(p), \quad u_{B}(p) = \frac{c\sigma.p}{E + mc^{2}} u_{A}(p).....3.113$$

Eliminating $u_B(p)$, we have

$$\Rightarrow \left(E^2 - m^2 c^4\right) u_A(p) = \left[c^2 p^2 + c\sigma(p \times p)\right] u_A(p)$$

$$\Rightarrow \left(E^2 - m^2 c^4\right) u_A(p) = c^2 p^2 u_A(p), \dots 3.115$$

since $p \times p = 0$

Similarly, upon elimination of $u_A(p)$, we also have

Hence the four eigenvalues of equation (3.111) are therefore given by

$$E_{+} = + \left(m^{2}c^{4} + p^{2}c^{2}\right)^{\frac{1}{2}} \quad occurring \ twice \ \dots \ 3.117a$$

and

For $E_{+} = +(m^2c^4 + p^2c^2)^{\frac{1}{2}}$, part from the normalization constant,

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} and \begin{pmatrix} 0 \\ 1 \end{pmatrix} for \ u_A(p) \dots 3.118$$

There are two linearly independent solutions for equation (3.111), corresponding to

the positive energy $E_{+} = +(m^2c^4 + p^2c^2)^{\frac{1}{2}}$, which describe a free $spin - \frac{1}{2}$ particle of

energy E_+ and momentum **p**. If we write

then the independent solution for E_+ or E > 0 are

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written as

$$u^{(1)}(p) = N \begin{pmatrix} 1 \\ 0 \\ p_{3}c/(E+mc^{2}) \\ (p_{1}+ip_{2})c/(E+mc^{2}) \end{pmatrix} , \quad u^{(2)}(p) = N \begin{pmatrix} 0 \\ 1 \\ (p_{1}-ip_{2})c/(E+mc^{2}) \\ -p_{3}c/(E+mc^{2}) \end{pmatrix} . \dots 3.120$$

For $E_{-} = -(m^2c^4 + p^2c^2)^{\frac{1}{2}} < 0$, we may start with the lower two-component spinor $u_B(p)$ set to

$$\begin{pmatrix} 1 \\ 0 \end{pmatrix} and \begin{pmatrix} 0 \\ 1 \end{pmatrix} for u_B(p) \dots 3.121$$

There are again two linearly independent solutions of this type, which may be written as

$$u^{(3)}(p) = N \begin{pmatrix} -p_3 c / ||E| + mc^2 \\ -(p_1 + ip_2) c / ||E| + mc^2 \\ 1 \\ 0 \end{pmatrix}, u^{(4)}(p) = N \begin{pmatrix} -(p_1 - ip_2) c / ||E| + mc^2 \\ p_3 c / ||E| + mc^2 \\ 0 \\ 1 \end{pmatrix} \dots 3.122$$

where N is the normalization constant.

3.9 Simple Solutions; Non-Relativistic Approximations; Plane Waves

3.9.1 Large and small components:

Before we study the behaviour of Dirac wave function Ψ under Lorentz

transformations, let us examine the kind of physics buried in the harmless-looking equation (3.76b).

In the presence of electromagnetic couplings, the Dirac equation reads

$$\left(\frac{\partial}{\partial x_{\mu}} - \frac{ie}{\hbar c} A_{\mu}\right) \gamma_{\mu} \Psi + \frac{mc}{\hbar} \Psi = 0 \dots 3.123$$

where the usual replacement $-i\hbar(\partial/\partial x_{\mu}) \rightarrow -i\hbar(\partial/\partial x_{\mu}) - eA_{\mu}/c$ is assumed to be valid. Assuming that A_{μ} is the time independent, we let the time dependence of Ψ be given by

which means that Ψ is an eigenfunction of $i\hbar\partial/\partial t$ with eigenvalue *E*.

From equation (3.121), we can then write the coupled equations for the upper and lower components, Ψ_A and Ψ_B as follows.

$$\Rightarrow -i\hbar(\partial/\partial x_{0})\Psi_{A} - i\hbar\sigma.\nabla\Psi_{B} = -mc\Psi_{A}$$

$$\Rightarrow -i\hbar\sigma.\nabla\Psi_{B} = (i\hbar(\partial/\partial x_{0}) - mc)\Psi_{A}.....3.125a$$

$$\Rightarrow i\hbar(\partial/\partial x_{0})\Psi_{B} + i\hbar\sigma.\nabla\Psi_{A} = -mc\Psi_{B}$$

$$\Rightarrow i\hbar\sigma.\nabla\Psi_{A} = -(i\hbar(\partial/\partial x_{0}) + mc)\Psi_{A}....3.125b$$

Substituting $i\hbar(\partial/\partial x_0) = E \rightarrow E - eA_0$ and $-i\hbar\nabla = p \rightarrow p - \frac{eA}{c}$ into equation

(3.125a) and (3.125b) we have (3.126a) and (3.126b).

.

where $A_{\mu} = (A, iA_0)$. Using equation (3.126b), we can readily eliminate Ψ_B in

equation (3.126a) to obtain

Up to now, we have made no approximations. We now assume that

Defining the energy measured from by

From equation (3.126), we can make the following expansion:

Equation (3.130) can be regarded as an expansion in powers of $(v/c)^2$ since $E^{(NR)} - eA_0$ is roughly

Keeping only the leading term in (3.130), we obtain

Using equation (3.76b), equation (3.132) then becomes

Thus to zeroth order in $(v/c)^2$, Ψ_A is nothing more than the Schrödinger-Paulo two component wave function in non-relativistic quantum mechanics multiplied by a factor $e^{-imc^2/\hbar}$. Using equation (3.126b), we see that Ψ_B is "smaller" than Ψ_A by a factor roughly $[\vec{p} - (eA/c)]/2m \approx v/2c$ provided that equation (3.128) is valid. For this reason with $E \approx mc^2$, Ψ_A and Ψ_B are respectively known as the large and small components of the Dirac wave function Ψ .

Chapter Four

Main Results

Non-homogeneous Klein-Gordon Equation with interacting term

This chapter stipulates the main findings. In it, the free particle Klein-Gordon equation became a non-homogenous equation, with the introduction of a n interacting term, which is a slow varying wave field, on the right hand side. Other sub-topics treated were the effects of the slow varying wave field interacting with the Schrodinger equation and Klein-Gordon equation. Annihilation and creation operators were also tackled.

4.1 Slow varying wave field

A field is said to be slow varying field if it has a low frequency. If we take for instance $\cos kx$ as a periodic function, when k is small, then the variation of $\cos kx$ will be slow and $\cos kx$ may be expanded as

4.2 Effects of slow varying wave field on the Schrodinger equation

4.2.1 Schrodinger Equation (Homogenous)

The non-homogenous relationship between the energy \vec{E} and the momentum \vec{p} of a free particle of spin 0 and the rest mass *m* are given:

$$\vec{E} = \frac{\vec{p}}{2m} \dots 4.2a$$

quantum mechanically by

$$\vec{E} \to i\hbar \frac{\partial}{\partial t}, \qquad \vec{p} \to i\hbar \nabla \dots 4.2b$$

The Schrodinger equation for a free particle is given by

$$\nabla^{2}\Psi + \frac{2m}{\hbar}E\Psi = 0 \dots 2.7b$$

$$\Rightarrow \nabla^{2}\Psi + \mu^{2}\Psi = 0 \dots 2.7c$$

$$\mu^{2} = \frac{2m}{\hbar}E$$

where

4.2.2 Schrodinger Equation (Non-Homogenous)

We want to look at cases when the free particle Schrodinger equation is replaced with forced term $-\kappa^2 \cos(kx)\Psi$. That is, if we replace the Right Hand Side of equation (2.7c) by the slow wave field, we have $\Rightarrow \nabla^2 \Psi + \mu^2 \Psi = -\kappa^2 \cos(kx)\Psi$4.3a

Substituting the expanded form of equation (4.1) into (4.3a), we have

Case I

When the right hand side of equation (4.3b) is approximated with the zero order term $-\kappa^2$, we will have

$$\nabla^2 \Psi + \mu^2 \Psi = -\kappa^2 \Psi \qquad4.4a$$
$$\nabla^2 \Psi + (\mu^2 + \kappa^2) \Psi = 0 \qquad4.4b$$

We may therefore write equation (4.4b) as

where

$$\gamma^2 = \mu^2 + \kappa^2$$

Case II

We want to also consider replacing the Right Hand Side of equation (4.5) with the

second order term $\frac{\kappa^2 x^2}{2}$, we will have

Equation (4.6) is the quantum simple Harmonic oscillator.

4.3 Effect of the slow varying wave field on the Klein-Gordon Equation

4.3.1 Klein-Gordon Equation (Homogenous)

The relativistic relationship between the energy \vec{E} and the momentum \vec{p} of a free

particle of spin 0 and the rest mass m is given

classically by

$$\vec{E}^2 = c^2 \vec{p}^2 + m^2 c^4 \dots 4.7$$

quantum mechanically by

$$\vec{E} \to i\hbar \frac{\partial}{\partial t}, \qquad \vec{p} \to i\hbar \nabla \dots 4.2b$$

If we quantize the relativistic equation (4.7), we have

$$\left[\hbar^2 \left(\frac{\partial^2}{\partial t^2} - c^2 \nabla^2\right) + m^2 c^4\right] \Psi = 0 \dots 4.8a$$

$$\Box^2 \Psi + \frac{m^2 c^4}{\hbar^2} \Psi = 0 \dots 4.8b$$

 $\Box^2 \Psi + \upsilon^2 \Psi = 0 \dots 4.8c$

Where
$$\square^2$$
 is the d'Alembertian operator and $\upsilon^2 = \frac{m^2 c^4}{\hbar^2}$

Equation (4.8c) is the Klein-Gordon equation for a free particle.

4.3.2 Klein-Gordon Equation (Non-Homogenous)

If the Right Hand Side of equation (4.8c) is replaced with a slow varying wave field (4.1), we will have

$$\Box^{2}\Psi + \upsilon^{2}\Psi = -\kappa^{2}\cos(kx)\Psi \dots 4.9a$$
$$\Rightarrow \Box^{2}\Psi + \upsilon^{2}\Psi = -\kappa^{2}\left(1 - \frac{k^{2}x^{2}}{2} + \dots\right)\Psi \dots 4.9b$$

Case I

If the right hand side of equation (4.9b) is replaced with the zero order term $-\kappa^2$, equation (4.6b) will become

Equation (4.10a) may be written as

 $\chi^2 = \upsilon^2 + \kappa$

$$\int^{2} \Psi + (\upsilon^{2} + \kappa^{2}) \Psi = 0 \dots 4.10b$$

$$\Rightarrow \Box^2 \Psi + \chi^2 \Psi = 0.....4.10c$$

where

Case II

If we also consider replacing the Right Hand Side of equation (4.10c) by the second order term, we will have

Now, the time independent Klein-Gordon equation may be written as

Where

Equation (4.12b) is called the relativistic Quantum Harmonic Oscillator

Equation (4.12b) is analogous to the Energy generated by the simple Harmonic oscillator, whose energy is given by

From equation (*), if $E^2 \square v^2$, then we can assume that

where η is new mass energy which represent the mass of the energy levels

produced by the Klein-Gordon equation.

If we equate equations (4.14) and (4.13), we have

$$u_n^2 = (2n+1)\frac{\hbar\omega}{2}$$
.....4.15a

$$\Rightarrow \mu_n = \pm \sqrt{(2n+1)\frac{\hbar\omega}{2}} \dots 4.15b$$

where

$$n = 0, 1, 2, \dots$$

Equation (4.15b) is generally the mass of the energy levels depicted by the Klein-Gordon equation. This equation shows the negative and positive masses of the energy levels indicated by the Klein-Gordon equation, which also represents the particles and antiparticles of the Klein-Gordon equation.

If n = 0, then equation (4.15b) becomes

Equation (4.16a) represents the mass of the energy level at the lowest state of the relativistic quantum harmonic oscillator.

When n = 1, equation (4.15b) then becomes

When n = 2, equation (4.15b) also becomes

Equations (4.16a,b&c) are the various energy levels, which indicate the downward and upward energy levels.

4.4 Dirac equation

For a Dirac solution of the non-homogeneous Klein-Gordon equation, we shall still make reference to equation (3.33) given by

$$\left[\hbar^{2}\left(\frac{\partial^{2}}{\partial t^{2}}-\nabla^{2}\right)+m^{2}\right]\Psi=i\hbar q(\vec{A}.\nabla+\Phi\frac{\partial}{\partial t})\Psi.....3.33a$$

Equation (3.33) may still be written as

We assume that

By writing equation (3.33b) in the Dirac representation and making use of equation

$$(4.19a)$$
, we have

$$\Rightarrow \left(i\hbar\frac{\partial}{\partial t} + \sigma.i\hbar\nabla\right) \left(i\hbar\frac{\partial}{\partial t} - \sigma.i\hbar\nabla\right) \Psi^{(L)} = i\hbar q \left(\Phi i\hbar\frac{\partial}{\partial t} + A\sigma.i\hbar\nabla\right) \Psi^{(L)} - m^2 \Psi^{(L)} \dots 4.18a$$
$$\Rightarrow \left(i\hbar\frac{\partial}{\partial t} + \sigma.i\hbar\nabla\right) \left(i\hbar\frac{\partial}{\partial t} - \sigma.i\hbar\nabla\right) \Psi^{(L)} = i\hbar q \Phi \left(i\hbar\frac{\partial}{\partial t} - \sigma.i\hbar\nabla\right) \Psi^{(L)} - m^2 \Psi^{(L)} \dots 4.18b$$

Set

$$\left(i\hbar\partial/\partial t - \sigma.i\hbar\nabla\right)\Psi^{(L)} = \Psi^{(R)}$$
.....4.19a

$$\Rightarrow \left(\sigma.i\hbar\nabla + i\hbar\partial/_{\partial t} - i\hbar q\Phi\right)\Psi^{(R)} = -m^2\Psi^{(L)} \qquad (4.19b)$$

We want to again assume that

$$\vec{A}\Psi = \Phi\Psi$$
4.17b

Substituting equation (4.17b) into equation (4.18a), we have

-

Setting

$$\left(i\hbar\partial/\partial t + \sigma \cdot i\hbar\nabla\right)\Psi^{(R)} = \Psi^{(L)}$$
.....4.21a,

$$\Rightarrow \left(i\hbar \frac{\partial}{\partial t} - \sigma . i\hbar \nabla - i\hbar q \Phi\right) \Psi^{(L)} = -m^2 \Psi^{(R)} \dots 4.21 b$$

To bring it to form originally written by Dirac, we will take the sum and difference of equations (4.19b & 4.21b). This gives us

$$-i\hbar \frac{\partial}{\partial t} \left(\Psi^{(R)} - \Psi^{(L)} \right) - \sigma .i\hbar \nabla \left(\Psi^{(R)} + \Psi^{(L)} \right) + i\hbar q \Phi \left(\Psi^{(R)} + \Psi^{(L)} \right) = -m^2 \left(\Psi^{(R)} - \Psi^{(L)} \right) \dots 4.22a$$
$$-i\hbar \frac{\partial}{\partial t} \left(\Psi^{(R)} + \Psi^{(L)} \right) - \sigma .i\hbar \nabla \left(\Psi^{(R)} - \Psi^{(L)} \right) - i\hbar q \Phi \left(\Psi^{(R)} - \Psi^{(L)} \right) = m^2 \left(\Psi^{(R)} + \Psi^{(L)} \right) \dots 4.22b$$

Denoting the sum and difference of $\Psi^{(R)}$ and $\Psi^{(L)}$ by ϕ_A and ϕ_B , we have

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$$-i\hbar\partial/\partial_t\phi_A - \sigma.i\hbar\nabla\phi_B - i\hbar q\Phi\phi_B = m^2\phi_A \dots 4.23b$$

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From equation (4.21a), we have

Making use of the total energy E and the momentum p as represented by the

differential operators,

$$E = i\hbar \partial/\partial t$$
 and $p = -i\hbar \partial/\partial x$2.25,

equation (4.24a) may be written as

By re-arrangement of terms, we have

$$(\sigma.p+i\hbar q\Phi)\phi_A = (E-m^2)\phi_B$$
.....4.24c

In a similar development and by way of considering equation (4.23b), we have

$$-i\hbar\partial/\partial t \phi_A + (-\sigma.i\hbar\nabla - i\hbar q\Phi)\phi_B = m^2\phi_A \dots 4.25a$$

substituting equation (2.13) into (4.25b), we have

$$-E\phi_A + (\sigma \cdot p - i\hbar q\Phi)\phi_B = m^2\phi_A \dots 4.25b$$

By re-arrangement of terms, we have

$$(\sigma \cdot p - i\hbar q\Phi)\phi_B = -(E + m^2)\phi_A$$
.....4.25c

The product of equation s (4.24c & 4.25c) may be written as

Where

Equation (4.26b) may be intuitively written as

Equation (4.26c) is of the form of the relativistic quantum harmonic oscillator.

In addition, equation (4.26c) can also be written as

Equation (4.26d) is also analogous with the Klein-Gordon equation.

We can also write the matrix representation of equations (4.24a & 4.25a) as

4.5 Annihilation and Creation operators

White (1966) deduced the annihilation and creation operators for the simple harmonic oscillator. Based on his assumptions, if we consider equations (4.24c and 4.25c), we can define two operators a and a^{\dagger} such that

$$a^{\dagger} = \frac{1}{\sqrt{2}} \left(\sigma. p + i\hbar q \Phi \right) \dots 4.28a$$
$$a = \frac{1}{\sqrt{2}} \left(\sigma. p - i\hbar q \Phi \right) \dots 4.28 \mathrm{b}$$

Equations (4.28) may be written as

$$\sqrt{2} a^{\dagger} \phi_{A} = \left(E - m^{2}\right) \phi_{B} \dots 4.29a$$

If we form the product operators

$$aa^{\dagger} = \frac{1}{2} \Big[(\sigma.p)^2 - i(\sigma.p - q\Phi) + (q\Phi)^2 \Big] \dots 4.30a$$

and

$$a^{\dagger}a = \frac{1}{2} \Big[(\sigma.p)^2 + i(\sigma.p - q\Phi) + (q\Phi)^2 \Big] \dots 4.30b$$

We observe that

Equation (4.31a) is the Hamiltonian operator of the relativistic harmonic oscillator in terms of a and a^{\dagger} operators.

Further, we note that

$$(aa^{\dagger} - a^{\dagger}a) = \frac{1}{2}(-2i)[\sigma \cdot p(q\Phi) - q\Phi(\sigma \cdot p)] \dots 4.31b$$
$$= -i[\sigma \cdot p, q\Phi]$$

 $=(-i)(i\hbar)$

$$\begin{bmatrix} a, a^{\dagger} \end{bmatrix} = \hbar \dots 4.32$$

a and a^{\dagger} operators obey a particularly simple commutation relation. Since, from this commutation rule,

$$aa^{\dagger} = \hbar + a^{\dagger}a \dots 4.33,$$

the modified Hamiltonian operator for the relativistic harmonic oscillator may be written as

$$= \frac{1}{2} (aa^{\dagger} + a^{\dagger}a) \dots 4.34$$
$$= \frac{1}{2} (2a^{\dagger}a + \hbar)$$
$$= (a^{\dagger}a + \frac{\hbar}{2}) \dots 4.35$$

Defining a new operator N such that

 $N=a^{\dagger}a\,,$

The Hamiltonian operator for the relativistic quantum harmonic oscillator will also become

$$H_{op} = \left(N + \frac{1}{2}\right)\hbar\omega \dots 4.36$$

We want to proceed by finding the eigenvalues and eigenfunctions for the Hamiltonian operator. Let us denote the eigenfunction by $|v\rangle$ such that

$$N|v\rangle = v|v\rangle$$
.....4.37

The symbol $|\rangle$ is called a ket; its dual $\langle |$ is called a bra. Together, the two symbols define a scalar product, which Dirac calls bracket $\langle | \rangle$. We want to derive the allowed values of υ by examining the relations between eigenfunctions implied by the Hamiltonian equation (4.37) and by the commutation relation between a and a^{\dagger} . To develop this relation between the eigenfunctions, we need to first develop two operator equalities involving Na and Na^{\dagger} .

$$Na = a^{\dagger}aa$$

$$= (aa^{\dagger} - 1)a$$

$$= aa^{\dagger}a - a$$

$$= a(a^{\dagger}a - 1)$$

$$= a(N-1).....4.38$$
and
$$Na^{\dagger} = a^{\dagger}aa^{\dagger}$$

$$= a^{\dagger}(a^{\dagger}a + 1)$$

$$= a^{\dagger}(N+1).....4.39$$

We now want to consider the vector $|v\rangle$ with *a*. Using the identity equation (4.38),

we find that

We can deduce from equation (4.40) that $a|v\rangle$ is an eigenvector of N belonging to

the eigenvalue v - 1.

Similarly,

$$Na^{\dagger} | \upsilon
angle = a^{\dagger} (N+1) | \upsilon
angle$$

 $= a^{\dagger} (\upsilon+1) | \upsilon
angle$

a and a^{\dagger} are respectively called the demotion (annihilation) and promotion (creation) operators.

a operating on the eigenfunction $|v\rangle$ demotes it to the eigenfunction belonging to the eigenvalue v-1, and a^{\dagger} operating on $|v\rangle$ promotes it to the eigenfunction belonging to the eigenvalue v+1.



Chapter Five

Conclusions

In this chapter, the summary of the results were given, followed by the conclusions, recommendations and suggestion for further research of the study. The study investigated the behaviour of the free particle Klein-Gordon equation when an interacting term is introduced on the right hand side of the equation. The interacting term which was a potential field was the slow varying periodic wave field, which contained the zero order and the second order approximations. It was found that when the zero order approximation was introduced at the right hand side of the equation, there was a shift in the mass energy. On the other hand, positive and negative energy masses, which also represent particles and antiparticles were obtained when the right hand side of the equation was replaced with the second order term. Annihilation and creation operators, which resulted in the formation of eigenvalues, were also realized. This became possible when the non-homogenous Klein-Gordon equation was solved by the Dirac format.

5.1 Summary of results

From the study, the relativistic Quantum mechanics for homogenous Klein-Gordon equation for free particles which is also a second order differential equation was reviewed.

Dirac equation which also extended the results to first order differential equation was also reviewed.

Dirac was able to shows that spinols are not only particles but there are antiparticles available.

The non-homogenous Klein-Gordon equation of the relativistic quantum mechanics was also reviewed. Only the space part was considered. In this regard, the interacting term of the Klein-Gordon equation was regarded as the forced particle. This led us to the relativistic quantum harmonic oscillator.

From the result, when the zero order term was replaced at the interacting term of the Klein-Gordon equation, it only introduced a shift in the mass, which did not lead to any significant change. On the other hand, when the interacting term of the Klein-Gordon equation was replaced with the quadratic term, positive, zero and negative masses of the energy, which represent the particles and antiparticles, were realized. Additionally, when the Klein-Gordon equation is written in Dirac format, there was the formation of creation and annihilation of eigenvalues and eigenfunctions.

5.2 Conclusion

We can therefore conclude that

1. The homogeneous Klein-Gordon equation and the corresponding Dirac Equation have been adequately been reviewed.

2. The non-homogeneous Klein Gordon equation with a slow varying wave field as the interacting term on the right hand side has also been thoroughly studied.

5.2 Recommendations

We recommend that physical interpretations and applications to this study be carried out.

It is also recommended that further investigation could be carried out on higher order approximations of the interacting slow varying wave field which leads to quantum anharmonic oscillators.

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