Dr. Cattani

Thank you for your kind note.
I hope it can be of some use to you.
Best wishes,
John R Fanchi
3/1/82

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ABSTRACT

QUANTUM MECHANICS OF RELATIVISTIC SPINLESS PARTICLES

BY

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A quantum mechanical theory of relativistic spinless particles, based upon the Born interpretation of the wavefunction, is constructed on $L^2(\vec{x},ct)$. A generalized Schrödinger equation is derived having a Hermitian Hamiltonian and the concept of superposition of mass states is introduced. Charge conjugation is discussed and a non-trivial framework for charged and neutral particles is provided. The Klein paradox is resolved and an experiment is suggested. A direct test of the theory is presented.

PREFACE

There are a number of ways to motivate the research embodied in this paper. My principal motivation for undertaking this work was the desire to answer the question: can free will and determinism coexist? The answer to this question has important consequences in fields other than physics, e.g. theology and economics.

Physics of the early twentieth century provided the answer "yes" to the above question in the following sense. Non-relativistic quantum mechanics, via the uncertainty principle and the Born interpretation, implied that the evolution of individual particles could not be predetermined on the microscopic level. Yet, on the average, the motion of an ensemble of particles could be accurately predicted. In other words, a 'free will'--a lack of predestination--exists in Nature on the microscopic level for the individual particle while, concurrently, determinism exists in Nature on the macroscopic level for an aggregate of particles. This was a major break from the concept of Newtonian determinism.

More recently, the difficulties associated with constructing a consistent theory of relativistic phenomena which employs a probabilistic basis have cast doubts on the answer "yes" to the question posed heretofore. The purpose of this research is to construct a quantum mechanical description of relativistic spinless particles that consistently utilizes probabilistic concepts. By achieving this goal one removes the doubts alluded to earlier and, consequently, gives additional credibility to the answer "yes", i.e. free will and determinism <u>can</u> coexist in Nature.

Before proceeding further I would first like to acknowledge: my wife, Katherine, for her support and patience; my adviser, R. Eugene Collins, for his physical insight, guidance, and professionalism; and, of course, my parents, John A. and Shirley, without whom this work would not have been possible.

TABLE OF CONTENTS

I. INTRODUCTION

The primary purpose of this research is to construct a consistent single-particle theory of relativistic spinless particles. The reasons such a theory does not already exist will be examined in this chapter. The new theory will then be presented in Chapter II. Chapters III - VI will examine the new theory and show how it can be used to resolve the difficulties associated with conventional theories.

A. History

In 1926 Schrödinger[1] introduced the concepts of wave mechanics to the scientific community. His work laid the foundation for non-relativistic quantum mechanics (NRQM). Let us record here three important relations of NRQM:

1) Schrödinger's equation

$$i\hbar \frac{\partial \psi_s}{\partial t} = \frac{-\hbar^2}{2m} \nabla^2 \psi_s + V \psi_s \ ; \tag{1.1}$$

2) the probability density

$$\rho_s = \psi_s^* \psi_s \geq 0 ; \tag{1.2}$$

and

3) the normalization condition

$$\int \rho_s \, d^3x = 1 \ . \tag{1.3}$$

Shortly after Schrödinger's first paper on NRQM there appeared the following equation[2-4]:

$$\left[\frac{\hbar}{i}\frac{\partial}{\partial x_\mu} - \frac{e}{c}A^\mu\right]\left[\frac{\hbar}{i}\frac{\partial}{\partial x^\mu} - \frac{e}{c}A_\mu\right]\psi = m_o^2 c^2 \psi \qquad (1.4)$$

where m_o is the rest mass of the particle*. Initially Eq. (1.4), now known as the Klein-Gordon (KG) equation, was thought to be the wave equation for relativistic particles. This belief was short-lived however.

From Eq. (1.4) and its complex conjugate one can derive the continuity equation

$$\frac{\partial j^\mu}{\partial x^\mu} = 0 \qquad (1.5)$$

where

$$j^\mu = \frac{-i\hbar}{2m_o}\left[\psi^* \frac{\partial \psi}{\partial x_\mu} - \psi \frac{\partial \psi^*}{\partial x_\mu}\right] - \frac{eA^\mu}{m_o c}\psi^*\psi. \qquad (1.6)$$

A continuity equation, having the form of Eq. (1.5) but with j^μ defined differently, could also be derived from Schrödinger's equation. In an effort to mimic the successful NRQM, it was assumed that j^0/c should be interpreted as the relativistic probability density. This assumption gave rise to problems of interpretation because j^0 could have negative values. Consequently the KG equation was considered inadequate as a wave equation for relativistic particles and an alternative was sought.

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* See Appendix A for details regarding notation and the metric.

Dirac's[5] relativistic theory was published a couple of years after the KG equation first appeared. The capability of the Dirac equation to accurately describe the electron, including the magnetic moment of the electron, quickly gained it acceptance as the proper description of relativistic particles. The KG equation was resurrected only after Pauli and Weisskoph[6] reinterpreted Eq. (1.4) as the field equation for spinless particles in the formalism of second quantization. They did not, however, resolve the problem of a 'negative probability density'.

Relativistic spinless particles (RSP) did receive some attention in later years in, for example, such notable papers as those of Wigner[7] and Bhabha[8], but the failings of the theories purporting to describe RSP were not eliminated.

Considerable interest in the theoretical description of RSP was generated when Lattes, et al.[9], discovered the pion in 1947. Eleven years later Feshbach and Villars[10] published a review article which discussed the properties of RSP as they were understood by the scientific community prior to 1958.

Today there exist essentially two points of view regarding the theoretical description of RSP by a single-particle theory. The most prominent is the two-component formalism whose foundation was first laid by Feshbach and Villars[10]. More recent discussions are given by Bjorken and Drell[11], and Baym[12]. The other formalism, as described by Schweber[13], assumes that the only physically realizeable energies of a free particle are those which are positive. These two theories will be referred to below as "conventional theories".

Though by no means exhaustive, this sketch does provide a backdrop for a more detailed discussion of the difficulties associated with the conventional theories.

B. Difficulties with Conventional Theories

The first difficulty to be described is that which was also the first recognized historically, namely negative probability densities. If the solution to the KG equation has a time dependence given by $e^{i\omega t}$, then j^0/c has the form

$$\frac{j^0}{c} = \frac{\hbar\omega - eA^0}{m_0 c^2}\,\psi^*\psi \tag{1.7}$$

The quantity j^0/c is negative whenever $\hbar\omega - eA^0$ is negative. Thus, by identifying j^0/c as a probability density, one encounters the difficulty of negative probability densities. The concept of a negative probability density was so unconventional when it was first introduced that the entire theory was considered inadequate. Only when Pauli and Weisskoph resurrected the KG equation did people begin to reassess the meaning of j^0/c. The two-component formalism of Feshbach and Villars is one such attempt.

In this theory one transforms the second-order KG equation into two first-order equations. One then attempts to separate the positive and negative energy components of the solution to the KG equation and then attach a positive and negative norm respectively. This is only possible, however, for weak, slowly varying potentials; otherwise the Hamiltonian, obtained by applying the Foldy-Wouthuysen transformation[14], will not converge or else will not be Hermitian. Thus the two-component formalism, for which a positive-definite probability density can be defined, is only an <u>approximate</u> formalism.

Alternatively, one can simply accept negative probability densities and disregard mathematical custom. In this case, that of accepting j^0/c as the probability density, one would define, say, the expectation value of a radius r as

$$\langle r \rangle = \frac{\int r \, j^0/c \, d^3x}{\int j^0/c \, d^3x} \tag{1.8}$$

which is what conventional theories do. An example will be given later which shows that Eq. (1.8) does not generally agree, in the non-relativistic limit, with the corresponding expectation value found using NRQM. This lack of agreement casts doubt on the validity of identifying j^0/c as a probability density and is a second difficulty which needs resolution.

Another approach to the problem of interpreting j^0/c is to assert that one must multiply j^0/c by the charge, e, of a particle in order to get a meaningful quantity. This quantity, ej^0/c, is then interpreted as the charge density. Thus the continuity equation, Eq. (1.5), upon multiplication by e represents the conservation of charge. This is certainly a non-trivial approach to the problem for charged particles. However for neutral particles, such as the neutral pion, multiplying by the charge is nothing more than multiplying by zero and Eq. (1.5) is converted into the trivial identity $0 = 0$. The fact that Eq. (1.5) is valid for neutral particles, i.e. j^0/c is conserved for neutral particles, suggests that the interpretation of j^0/c is not yet complete. Finding an interpretation of j^0/c which is non-trivial for both charged <u>and</u> neutral particles is a new, a third, difficulty which must be confronted. This point has recently been acknowledged by Marx[15].

The three difficulties mentioned heretofore are based on two facts: the existence of positive and negative energy solution; and the existence of a continuity equation for j^μ. These facts are responsible for two more difficulties.

The existence of negative energy solutions was a difficult concept to accept when it was first recognized. When Dirac found that his formalism also required the existence of negative energy solutions, his explanation was the, now well known, hole theory[16]. The hole theory, based on the Pauli exclusion principle, was, and is, quite suitable for fermions. However for bosons, such as the RSP considered here, the hole theory is useless. Eleven years later Stückelberg suggested the interpretation that positive energy solutions represent particle propagation forward in time and negative energy solutions represent particle propagation backward in time. This interpretation, adopted by Feynman[18] in his development of propagator theory, seems to have resolved the difficulty of understanding the negative energy solutions; however, this interpretation is, at present, only an ad hoc addition to conventional theories. Furthermore, this interpretation preserves the single-particle character of conventional theories, an achievement Dirac's hole theory cannot claim. It will be an asset for any single-particle theory of RSP if that theory includes, as an integral part, the Stückelberg-Feynman interpretation.

It has already been pointed out that j^0/c has not yet been adequately interpreted, but now it will be shown that even the interpretation of j^0/c as a charge density is not without problems. This difficulty, first introduced by Klein[19] and now known as the Klein paradox, arises when the problem of scattering from a step potential is considered. Using the interpretation of ej^0/c as the charge density Klein and, more recently, Winter[20] have shown that the reflection coefficient for an incident RSP will actually exceed unity. This prediction has no foundation in experimental fact and comprises a fourth difficulty of conventional theories.

A fifth difficulty of conventional theories is that a correspondence to relativistic classical
7 mechanics cannot be made from the KG equation because the relativistic classical equation of motion does not have a quantum analog.

The sixth, and final, difficulty to be discussed here is that unstable particles cannot be consistently described by conventional theories. This is so because conventional theories assume that probability is conserved in space only, whereas unstable particles are describeable by marginal probability densities in time[22,23]. It may be that one should not expect single-particle theories to describe particle decay; however, this point of view has not been proved. It must be recognized that any theory which purports to completely describe RSP is deficient if that theory cannot describe particle decay for the simple fact that RSP do decay. Thus a single-particle theory which can describe particle decay is more complete than those which cannot.

The situation has been summed up concisely by Schweber[13]: "A wholly consistent relativistic one-particle theory can be put forth only for free particles".

C. A Course of Action

The purpose of this thesis is to describe a consistent quantum mechanical theory of RSP which is free of the above difficulties. The approach to be employed parallels that developed by Collins[24,25] for NRQM and places probabilistic concepts at the foundation of quantum mechanics.

in what

Let us recall that the use of probabilistic concepts in NRQM has been successful. Historically the early relativistic quantum mechanical theories were, to a large extent, constructed in a manner analogous to their non-relativistic counterparts.

Two particularly important non-relativistic relations were Born's statistical interpretation of Ψ_S, Eq. (1.2), and the spatial normalization of the probability density, Eq. (1.3). It has been the custom in spinless-particle, relativistic, quantum theories to retain Eq. (1.3) and discard Eq. (1.2). Some of the difficulties mentioned above are a consequence of this procedure.

The approach taken here is to retain Eq. (1.2), so that a positive definite probability density, ρ, is assured, but to assume that ρ is a distribution in space and time. Thus it is necessary to abandon Eq. (1.3) and extend the normalization condition to include time as well. The implementation and interpretation of this program is the subject of the rest of this paper.

II. FOUR-SPACE FORMULATION

In order to treat space and time in an essentially symmetric way, the probability density ρ should represent a joint distribution in the space <u>and</u> time coordinates, though ρ may be conditioned by some invariant parameters. In particular it is postulated that ρ is conditioned by an invariant parameter τ. Then the conditional probability density is expressed as $\rho(\vec{x},ct|\tau)$, and the corresponding normalization condition is

$$\int_D \rho(\vec{x},ct|\tau)\, d^4x = 1\, ; \quad d^4x \equiv dx^0 dx^1 dx^2 dx^3 . \tag{2.1}$$

The quantity D is the domain of definition on which ρ may be non-zero, and $\rho(\vec{x},ct\,|\,\tau)dx^0d^3x$ is the probability that the particle is at the world-point $(\vec{x},ct)$ when the parameter has the value τ. Since a particle can occupy any world-point in space-time, it follows that D must extend over <u>all</u> of space and time.

The fact that the norm is a constant in Eq. (2.1) suggests that the density $\rho(\vec{x},ct|\tau)$ obeys a continuity equation in space-time. Preservation of the norm in four-space can be assured by requiring that $\rho(\vec{x},ct|\tau)$

in space-time; τ
$\frac{\partial\rho}{\partial\tau} + \mathrm{div}^4\, \rho\vec{V} = 0$

vanishes as $|x^\mu| \to \infty$ and obeys the equation

$$\frac{\partial}{\partial\tau} \rho(\vec{x}, ct|\tau) + \frac{\partial}{\partial x^\mu}\left[\rho(\vec{x}, ct|\tau) V^\mu\right] = 0 \qquad (2.2)$$

where V^μ is not yet defined. In this equation it is necessary that ρ and $\{V^\mu\}$ be single-valued and differentiable, and it is also <u>assumed</u> that the metric implied here is that of special relativity as defined in Appendix A.

Rather than simply assuming Eq. (2.2), one could have required that ρd^4x be invariant with respect to a five dimensional velocity field having as components $\{V^\mu\}$ and $V^4=1$, where a fifth coordinate x^4 is defined to be τ. The techniques of a procedure such as this are discussed by Kiehn[26], and it can be shown that Eq. (2.2) is one of two conditions for the invariance of ρd^4x with respect to propagation down the trajectories of $(\{V^\mu\}, V^4=1)$. The other condition is either $\partial V^\mu/\partial\tau$ is zero for all values of μ or $d\tau$ is zero. Either approach, simply assuming Eq. (2.2) is valid or else requiring ρd^4x to be invariant with respect to $(\{V^\mu\}, V^4=1)$, can be used here.

The physical meaning of the velocity field $\{V^\mu\}$ is determined by examining the expectation value of the space-time position vector of the particle,

$$\langle x^\mu \rangle = \int_D x^\mu \rho \, d^4x \, . \qquad (2.3)$$

Differentiating $\langle x^\mu \rangle$ with respect to τ ; substituting Eq. (2.2) for $\partial\rho/\partial\tau$, and applying the divergence theorem with the boundary condition that ρ vanishes as $|x^\mu| \to \infty$, yields

$$\frac{d}{d\tau}\langle x^\mu \rangle = \int_D V^\mu \rho \, d^4x. \qquad (2.4)$$

In other words, the expectation value of V^μ is the derivative, with respect to τ , of the expectation value of the four-position vector. This fact, along with Eq. (2.2), motivates the characterization of the quantities τ and $d\langle x^\mu \rangle/d\tau$ as statistical analogs of the classical proper-time and proper-velocity respectively. This characterization will be further justified below.

Now the Hilbert space formalism follows from this probabilistic description by first observing that, since ρ must be non-negative and differentiable, all derivatives of ρ must vanish when ρ vanishes, otherwise ρ would be somewhere negative. The Born representation is an acceptable mathematical form for assuring this constraint; thus write

$$\rho(\vec{x},ct|\tau) = \psi^*(\vec{x},ct,\tau)\,\psi(\vec{x},ct,\tau) \geq 0 \qquad (2.5)$$

where ψ and ψ^* are Lorentz invariant scalars. The function ρ satisfies the requirements of integrability, continuity, and differentiability if ψ is both Lebesque square integrable and differentiable. The quantity ψ has the form

$$\psi(\vec{x},ct,\tau) = \rho(\vec{x},ct|\tau)^{1/2}\, e^{i\phi(\vec{x},ct,\tau)} \qquad (2.6)$$

where ϕ is a real scalar function as yet undetermined.

The four-vector $\{V^\mu\}$ of Eq. (2.2) can always be written as

$$V^\mu = \frac{\hbar}{\bar{m}}\frac{\partial\phi}{\partial x_\mu} + \left[V^\mu - \frac{\hbar}{\bar{m}}\frac{\partial\phi}{\partial x_\mu}\right] \qquad (2.7)$$

where $\hbar/\bar{m}$ is an unspecified constant with units such that ϕ is dimensionless. One can then define

$$\epsilon A^\mu \equiv \left[V^\mu - \frac{\hbar}{\bar{m}}\frac{\partial\phi}{\partial x_\mu}\right] \qquad (2.8)$$

in terms of which Eq. (2.8) becomes

$$V^\mu = \frac{\hbar}{\bar{m}}\frac{\partial\phi}{\partial x_\mu} + \epsilon A^\mu \qquad (2.9)$$

Here ϵ is a constant setting the scale and units of A^μ. The quantity A^μ has the same harmonic and rotational parts as does V^μ, although their solenoidal parts may differ. Equation (2.9) expresses V^μ in terms of two quantities which depend on the phase of ψ. A relationship between A^μ, later to be identified as the four-vector potential of the electromagnetic field, and ϕ has been suggested before[27,28]. The consequence of Eq. (2.9) is the following.

The value of the density ρ is unchanged by the transformation

$$\psi' = \psi \exp\left[-i\frac{\epsilon\bar{m}}{\hbar}\Lambda\right] \qquad (2.10)$$

where Λ is a real scalar function of $(\vec{x},ct)$. This implies that ψ is specified only to within a gauge transformation of the first kind. The gauge transformation in Eq. (2.9) corresponds to the phase change

$$\phi' = \phi - \frac{\epsilon \bar{m}}{\hbar}\Lambda \tag{2.11}$$

and must be accompanied by the gauge transformation of the second kind

$$A'^{\mu} = A^{\mu} + \frac{\partial \Lambda}{\partial x_{\mu}} \tag{2.12}$$

so that Eq. (2.2) remains invariant with respect to the above transformations. The final result is that V^{μ} and ρ are unchanged by these gauge transformations, and one concludes that both A^{μ} and ψ are specified only to within a gauge transformation.

The function ϕ has a topological significance which will not be examined here (see Reference 28 for a brief discussion of the non-relativistic analog).

Using Eqs. (2.5) and (2.9) in Eq. (2.2) yields

$$\frac{\partial}{\partial \tau}\psi^*\psi + \frac{\partial}{\partial x^{\mu}}\left[\psi^*\left(\frac{\hbar}{\bar{m}}\frac{\partial \phi}{\partial x_{\mu}} + \epsilon A^{\mu}\right)\psi\right] = 0 . \tag{2.13}$$

Also from Eq. (2.6) there results

$$\frac{\partial \phi}{\partial x_{\mu}} = \frac{-i}{2\rho}\left[\psi^*\frac{\partial \psi}{\partial x_{\mu}} - \psi\frac{\partial \psi^*}{\partial x_{\mu}}\right] \tag{2.14}$$

which, when substituted into Eq. (2.12), yields

$$\frac{\partial}{\partial \tau}(\psi^*\psi) + \frac{\partial}{\partial x^{\mu}}\left[\frac{-i\hbar}{2\bar{m}}\left(\psi^*\frac{\partial \psi}{\partial x_{\mu}} - \psi\frac{\partial \psi^*}{\partial x_{\mu}}\right) + \epsilon A^{\mu}\psi^*\psi\right] = 0 . \tag{2.15}$$

Now this can be rearranged to read

$$\psi^* F = F^*\psi = (\psi^* F)^* \tag{2.16}$$

where the quantity F is

$$F = i\hbar\frac{\partial \psi}{\partial \tau} + \frac{\hbar}{2\bar{m}}\frac{\partial^2 \psi}{\partial x_{\mu}\partial x^{\mu}} - \frac{i\hbar}{2\bar{m}c}\left[\frac{\partial A^{\mu}\psi}{\partial x^{\mu}} + A^{\mu}\frac{\partial \psi}{\partial x^{\mu}}\right] . \tag{2.17}$$

This shows that the product $\psi^* F$ must be real and this is assured, for arbitrary ψ , if F has the form $U\psi$ with U a real scalar. The simplest possible form for U which keeps Eq. (2.17) gauge and Lorentz invariant is $e^2 A^\mu A_\mu / 2\bar{m}c^2$, where ϵ is now written as

$$\epsilon = -e/\bar{m}c \tag{2.18}$$

with e and c unspecified constants. The result is

$$i\hbar \frac{\partial \psi}{\partial \tau} = \frac{1}{2\bar{m}}\left[\frac{\hbar}{i}\frac{\partial}{\partial x_\mu} - \frac{e}{c}A^\mu\right]\left[\frac{\hbar}{i}\frac{\partial}{\partial x^\mu} - \frac{e}{c}A_\mu\right]\psi \tag{2.19}$$

$$\equiv p^\mu p_\mu \psi / 2\bar{m}$$

with $p^\mu p_\mu$ a scalar operator.

Equation (2.19) is a generalized form of the KG equation if A^μ is identified as the four-vector potential, c as the electric charge of the particle, $\bar{m}$ as a constant with mass units, $\hbar$ as Planck's constant divided by 2π , and c as the speed of light.

Equation (2.19) has the form of the Schrödinger equation except that Eq. (2.19) is defined on a four-space with a Lorentz metric. Since it does have the form of the Schrödinger equation many of the procedures and results of Schrödinger wave mechanics can be paralleled by the four-space formulation (FSF), although care must be exercised in working with the metric. This fact suggests that much of the effort needed to develop the FSF should be concentrated on interpretation because the appropriate mathematical techniques are already familiar from NRQM. Such will be the case below. Let it also be noted that the appearance of τ in Eq. (2.19) makes it possible to establish a correspondence between the relativistic classical and quantum theories.

The meaning of the operator p^μ in the formalism here is made clear by observing, in the manner of Collins[24] for the non-relativistic case, that if one inserts the above representations for V^μ and ρ in terms of ψ and A^μ into Eq. (2.4) for $d\langle x^\mu\rangle/d\tau$ there results

$$m \frac{d\langle x^\mu\rangle}{d\tau} = \int \psi^* \left[\frac{\hbar}{i}\frac{\partial}{\partial x_\mu} - \frac{e}{c} A^\mu \right] \psi \, d^4x = \langle p^\mu \rangle . \qquad (2.20)$$

This defines the expectation value of a relativistic "proper" momentum. From this definition of the momentum operator p^μ follow the familiar commutation rules for canonically conjugate coordinates and momenta and, from these, follow the corresponding uncertainty relationships, however the energy-time relationship is now on the same mathematical basis as the momentum-spatial coordinate relationships.

Direct generalization then yields the definition

$$\langle \Omega \rangle = \int \psi^* \Omega \psi \, d^4x \qquad (2.21)$$

for the expectation value of any observable associated with the particle, that is, the expectation value for any function of the x^μ or any derivative of such an expectation value, as p^μ above.

One can specify some boundary conditions on Ψ given some 'a priori' assumptions. Recalling that ρ and $\{V^\mu\}$ have been assumed single-valued and continuous, two particularly familiar boundary conditions are obtained by assuming that Ψ and $\{A^\mu\}$ are also single-valued and continuous. Integrating Eq. (2.2) over a "pillbox" in space-time, letting its length normal to the boundary go to zero, and employing the divergence theorem as in electrostatic theory[29] yields

$$-\frac{i\hbar}{2\bar{m}}\left[\Psi_I^* \frac{\partial \Psi_I}{\partial n} - \Psi_I \frac{\partial \Psi_I^*}{\partial n}\right] - \frac{eA_I^\mu}{\bar{m}c} n_\mu \rho_I \tag{2.22}$$

$$= -\frac{i\hbar}{2\bar{m}}\left[\Psi_{II}^* \frac{\partial \Psi_{II}}{\partial n} - \Psi_{II} \frac{\partial \Psi_{II}^*}{\partial n}\right] - \frac{eA_{II}^\mu}{\bar{m}c} n_\mu \rho_{II}$$

where $\partial/\partial n$ represents the normal derivative, n_μ is the unit normal vector, and all quantities are evaluated at the boundary between regions I and II.

Since Ψ is single-valued

$$\Psi_I = \Psi_{II} \tag{2.23}$$

on the boundary. Equations (2.22) and (2.23), with the fact that $\{A^\mu\}$ is single-valued, imply the other boundary condition, namely

$$\frac{\partial \Psi_I}{\partial n} = \frac{\partial \Psi_{II}}{\partial n} \, . \tag{2.24}$$

Equations (2.23) and (2.24) state that Ψ and its normal derivative are continuous at the boundary.

In addition to these conditions, one also observes that Ψ must vanish at any boundary where the four-vector potential has an infinite discontinuity. If this were not true, then the probability flux, $\{\rho V^{\mu}\}$, would be unbounded across the boundary.

III. GENERALIZED SCHRÖDINGER EQUATION

It is straightforward to prove that p^μ is Hermitian and, consequently, that $p^\mu p_\mu$ is also Hermitian. One can use this fact to write Eq. (2.19) as

$$i\hbar \frac{\partial \Psi}{\partial \tau} = H\Psi \; ; \; H \equiv \frac{1}{2m} p^\mu p_\mu \qquad (3.1)$$

where H is a Hermitian operator. Equation (3.1) is essentially a generalized Schrödinger equation. Since H is Hermitian, there exists a set of wavefunctions which constitutes a basis of eigenvectors for $L^2(\vec{x}, ct)$ obeying the orthonormality condition

$$\int \Psi_{q'}^* \Psi_q \, d^4x = \delta_{q'q} \qquad (3.2)$$

where Ψ_q is a solution of the equation

$$q \Psi_q = p^\mu p_\mu \Psi_q \, . \qquad (3.3)$$

The form of Eq. (3.3) suggests that q represents the square of an invariant momentum. Therefore let us define the magnitude of the expectation value of $p^\mu p_\mu$ as $m_o^2c^2$. This identification will be elaborated upon shortly. First observe that Eqs. (3.1) - (3.3) are valid whether potentials are present or not. Such orthonormality relationships cannot be consistently defined within conventional theories except for the free particle case. Furthermore, H is Hermitian regardless of the strength of the potentials. This is a claim that conventional theories, such as the two-component theory of Feshbach and Villars[10], cannot make because the KG equation with potentials is not, in general, diagonalizeable into separate positive- and negative-energy parts[11].

Given Eq. (3.1) a formalism is readily obtained which parallels non-relativistic Schrödinger theory. Tables 1 and 2 sketch this parallel explicitly. Table 1 shows the close similarity between the mathematical foundations of the relativistic and non-relativistic formalisms. The equations of motion in the Heisenberg picture for the non-relativistic and relativistic formalisms are compared in Table 2. One can see that there now exists a classical correspondence for the relativistic theory. Thus the results depicted in Table 2 eliminate the fifth difficulty described in Section I.B.

In spite of the mathematical similarities, there are concepts which have no parallel in the non-relativistic formalism. One such concept is the superposition of mass states.

The general solution of Eq. (3.1) is a superposition of the eigenfunctions, i.e.

$$\Psi(\vec{x},ct,\tau) = \sum_q A(q)\,\Psi_q(\vec{x},ct)\,\exp\left\{-\frac{iq\tau}{2m\hbar}\right\} \tag{3.4}$$

with A(q) denoting the expansion coefficients. Since both positive and negative values of q are admissable, it is possible for the expectation value of $p^\mu p_\mu$ to be negative; the FSF thus includes both tardyons and tachyons[30-34]. For tardyons,

$$\langle p^\mu p_\mu \rangle = m_0^2 c^2 \geq 0 \tag{3.5}$$

which is the special relativistic light cone constraint in energy-momentum space. Furthermore the general solution, Eq. (3.4), can now be thought of as a superposition of mass states, a concept that is mathematically similar to the non-relativistic concept of superposition of energy states. This interpretation will be discussed in more detail below for the free particle.

Table 1: Comparison of the Similarities Between Non-Relativistic Quantum Mechanics and the Four-Space Formulation

NON-RELATIVISTIC[a]		RELATIVISTIC
	Probability Density	
$\rho_N(\vec{x}\|t) = \Psi_N^*(\vec{x},t)\,\Psi_N(\vec{x},t)$		$\rho(\vec{x},ct\|\tau) = \Psi^*(\vec{x},ct,\tau)\Psi(\vec{x},ct,\tau)$
	Normalization	
$\int \rho_N\, d^3x = 1$		$\int \rho\, d^4x = 1$
	Continuity Equation	
$\frac{\partial \rho_N}{\partial t} + \nabla\cdot\vec{S} = 0$		$\frac{\partial \rho}{\partial \tau} + \frac{\partial}{\partial x^\mu} j^\mu = 0$
	Probability Flux	
$\vec{S} = \left(\frac{\hbar}{m}\nabla\phi_N - \frac{e}{mc}\vec{A}\right)\rho_N$		$j^\mu = \left(\frac{\hbar}{m}\frac{\partial\phi}{\partial x_\mu} - \frac{e}{mc}A^\mu\right)\rho$
	Differential Equation[b]	
$i\hbar\frac{\partial\Psi_N}{\partial t} = \frac{\vec{p}\cdot\vec{p}}{2m}\Psi_N + V\Psi_N$	where	$i\hbar\frac{\partial\Psi}{\partial\tau} = \frac{1}{2m}p^\mu p_\mu\Psi$
$\vec{p} = \frac{\hbar}{i}\nabla - \frac{e}{c}\vec{A}$		$p^\mu = +\frac{\hbar}{i}\frac{\partial}{\partial x_\mu} - \frac{e}{c}A^\mu$
	General Solution	
$\Psi_N(\vec{x},t) = \sum_E A_E(t_0)\,\Psi_E(\vec{x})\,e^{-iE(t-t_0)/\hbar}$	where	$\Psi(\vec{x},ct,\tau) = \sum_g A_g(\tau_0)\,\Psi_g(\vec{x},ct)\,e^{-\frac{i g_1(\tau-\tau_0)}{2m\hbar}}$
$A_E(t_0) = \int \Psi_E^*(\vec{x})\,\Psi_N(\vec{x},t_0)\,d^3x$		$A_g(\tau_0) = \int \Psi_g^*(\vec{x},ct)\,\Psi(\vec{x},ct,\tau_0)\,d^4x$
	Commutation Relations[c]	
$[\vec{x},\vec{p}] = i\hbar$ $[t, i\hbar\frac{\partial}{\partial t}] = -i\hbar$		$[x_\mu, p_\mu] = -i\hbar\, g_{\mu\mu}$
	Uncertainty Relations	
$\|\Delta\vec{x}\|\cdot\|\Delta\vec{p}\| \geq \frac{1}{2}\hbar$ $\|\Delta t\|\,\|\Delta E\| \geq \frac{1}{2}\hbar$		$\|\Delta x_\mu\|\,\|\Delta p_\mu\| \geq \frac{1}{2}\hbar$

a. See Schiff[35] for details regarding NRQM.
b. V is the potential energy.
c. A repeated index is not summed here. Also $g_{00} = 1 = -g_{11} = -g_{22} = -g_{33}$.

Table 2: A Classical Correspondence

NON-RELATIVISTIC[a]	RELATIVISTIC

Heisenberg Equation of Motion[b]

$$\frac{d}{dt}\omega'_{ij} = \left(\frac{\partial\Omega'}{\partial t}\right)_{ij} + \frac{1}{i\hbar}\left([\Omega',H']\right) \qquad \frac{d}{d\tau}\omega_{ij} = \left(\frac{\partial\Omega}{\partial\tau}\right)_{ij} + \frac{1}{i\hbar}\left([\Omega,H]\right)_{ij}$$

where

$$H' = \frac{1}{2m}\vec{p}\cdot\vec{p} + V \qquad H = \frac{1}{2m}p^{\mu}p_{\mu}$$

and

$$\omega'_{ij} = \int \Psi^*_{E_i}\Omega\Psi_{E_j}\,d^3x \qquad \omega_{ij} = \int \Psi^*_{\gamma_i}\Omega\Psi_{\gamma_f}\,d^4x$$

Classical Correspondence[c]

$$\{F,H'\} \to \frac{1}{i\hbar}[F,H'] \qquad \{\mathcal{F},H\} \to \frac{1}{i\hbar}[\mathcal{F},H]$$

where

$$[F,H'] = FH' - H'F \qquad [\mathcal{F},H] = \mathcal{F}H - H\mathcal{F}$$

and

$$\{F,H'\} = \sum_{j=1}^{3}\left[\frac{\partial F}{\partial x^j}\frac{\partial H'}{\partial P_j} - \frac{\partial H'}{\partial x^j}\frac{\partial F}{\partial P_j}\right] \qquad \{\mathcal{F},H\} = \frac{\partial\mathcal{F}}{\partial x^{\lambda}}\frac{\partial H}{\partial P_{\lambda}} - \frac{\partial H}{\partial x^{\lambda}}\frac{\partial \mathcal{F}}{\partial P_{\lambda}}$$

a. See Schiff[35] for details regarding NRQM.
b. $(A)_{ij}$ represents the ij^{th} matrix element of A.
c. $\{\}$ represents a Poisson bracket. The classical P_j's are defined by[21]

$$P_j \equiv \partial L/\partial u^j$$

where u^j is the three-(proper) velocity for the non-relativistic (relativistic) case, and L is the classical Lagrangian. In the corresponding quantum theory P_j is replaced by $\frac{\hbar}{i}\,\partial/\partial x^j$.

IV. CHARGED AND NEUTRAL PARTICLES: THE FREE PARTICLE AND CHARGE CONJUGATION

The free particle is defined by setting the four-vector $\{A^\mu\}$ to zero everywhere, or by setting the charge e to zero. Equation (2.19) becomes, with the metric now explicit,

$$+i\hbar \frac{\partial \Psi}{\partial \tau} = \frac{\hbar^2}{2m}\left[\nabla^2 - \frac{1}{c^2}\frac{\partial^2}{\partial t^2}\right]\Psi \tag{4.1}$$

with the general solution

$$\Psi(\vec{x},ct,\tau) = \iint_{-\infty}^{\infty}\left\{\frac{A(\vec{k},\omega)}{(2\pi)^4}\exp\left[\frac{i\hbar^2}{2m\hbar}\left(\vec{k}\cdot\vec{k} - \frac{\omega^2}{c^2}\right)\tau + i\left(\omega t - \vec{k}\cdot\vec{x}\right)\right]\right\} d^3k \, d\frac{\omega}{c} . \tag{4.2}$$

Here x^0 is expressed as ct. The notion of the direction of particle propagation in space and time can be thought of as follows.

Using Eq. (4.2) in Eq. (2.4) yields

$$\frac{d\langle x^\mu\rangle}{d\tau} = \frac{\hbar}{m}\langle k^\mu\rangle = \langle V^\mu\rangle \tag{4.3}$$

where the invariant interval $d\tau$ is taken to be positive. The space components of the quantity $\{V^\mu\}$ correspond to the space components of the phase velocity, and V^0 corresponds to the temporal component of the phase velocity which is interpreted as follows. If, in fact, a particle is progressing into the future when $d\langle ct\rangle$ is positive, and regressing into the past when $d\langle ct\rangle$ is negative, then

Eq. (4.3) says that a positive frequency wave propagates forward in time and a negative frequency wave propagates backward in time. This result parallels the Feynman-Stückelberg interpretation[17,18]. Furthermore, in the non-relativistic limit when $m_0^2 c^2 \gg \hbar^2 \langle \vec{k} \cdot \vec{k} \rangle$, one has

$$|\langle v^0 \rangle| \to c \tag{4.4}$$

as, indeed, it must.

The appearance of the Feynman-Stückelberg interpretation as an inherent part of the FSF is a significant achievement of the FSF for the reasons discussed in Section I.B. It is well to repeat here, however, that the Feynman-Stückelberg interpretation provides an acceptable physical interpretation of positive- and negative-energy solutions <u>within</u> the framework of single-particle theories such as the FSF. Thus it is <u>not</u> necessary, because of the existence of negative-energy solutions, to reinterpret the KG equation of the generalized Schrödinger equation, Eq. (3.1), as field equations which can be understood only within the framework of many-body theories. This is an important accomplishment which is readily applicable to the concept of charge conjugation.

The complex conjugate of Eq. (3.3) is

$$\left[i\hbar \frac{\partial}{\partial x^\mu} + \frac{e}{c} A_\mu\right]\left[i\hbar \frac{\partial}{\partial x_\mu} + \frac{e}{c} A^\mu\right] \psi_g^* = g\, \psi_g^* \tag{4.5}$$

where the quantity Ψ_q^* is the solution of the KG equation with the charge e replaced by -e. Thus the probability density remains unchanged with respect to charge conjugation. What does change?

If one writes Ψ_q as $Re^{i\Phi}$ then ρV^μ becomes

$$\rho V^\mu = \left[\frac{\hbar}{m}\frac{\partial \Phi}{\partial x_\mu} - \frac{eA^\mu}{mc}\right]R^2. \tag{4.6}$$

Replacing e by -e and interchanging Ψ_q with Ψ_q^* will change the sign of V^μ and $\langle V^\mu \rangle$. This says that a charged particle and its oppositely charged anti-particle propagate in opposite spatial and temporal directions for a given potential configuration. Feshbach and Villars[10] arrived at this interpretation by defining a 'negative probability density', but the FSF avoids this difficulty. It should also be noted that these remarks are applicable to the free particle solutions which, in turn, can be used to describe neutral particles. Thus a non-trivial interpretation of j^0/c can be provided for both charged and neutral particles by the FSF, thereby avoiding another difficulty of conventional theories.

Returning now to the free particle, let us observe that the rest mass of a free tardyon is given by Eq. (3.5), i.e.

$$m_0^2c^2 = \langle p^\mu p_\mu \rangle = \hbar^2\left[\left\langle \frac{\omega^2}{c^2}\right\rangle - \langle \vec{k}\cdot\vec{k}\rangle\right] \tag{4.7}$$

which is obtained by substituting Eq. (4.2) into Eq. (2.21) with Ω being $p^\mu p_\mu$. Thus one obtains the familiar relationship of relativity theory between energy, $\hbar\omega$, momentum, $\hbar\vec{k}$, and the observed rest mass in terms of espectation values. Equations (4.3) and (4.7) can be used to generate another significant result.

Integrating Eq. (4.3), for a small increment, $\delta\tau$, in τ, one finds

$$\delta\langle\vec{x}\rangle = \frac{\hbar}{\bar{m}}\langle\vec{k}\rangle\,\delta\tau \qquad \text{and} \qquad \delta\langle ct\rangle = \frac{\hbar}{\bar{m}}\left\langle\frac{\omega}{c}\right\rangle\delta\tau \tag{4.8}$$

where the space and time components have been separated and explicitly written. Forming the inner product of the four-vector $\{\delta(x^\mu)\}$ yields

$$\begin{aligned}\delta\langle x^\mu\rangle\,\delta\langle x_\mu\rangle &= (\delta\langle ct\rangle)^2 - \delta\langle\vec{x}\rangle\cdot\delta\langle\vec{x}\rangle \qquad (4.9)\\ &= \frac{\hbar^2}{\bar{m}^2}\left\{\left\langle\frac{\omega}{c}\right\rangle^2 - \langle\vec{k}\rangle\cdot\langle\vec{k}\rangle\right\}.\end{aligned}$$

Using Eq. (4.7) in Eq. (4.9) gives

$$\begin{aligned}(\delta\langle ct\rangle)^2 - \delta\langle\vec{x}\rangle\cdot\delta\langle\vec{x}\rangle \qquad (4.10)\\ = \frac{c^2 m_0^2\,\delta\tau^2}{\bar{m}^2} - \left[\frac{\Delta^2\omega}{c^2} - \Delta^2\vec{k}\right]\frac{\hbar^2\,\delta\tau^2}{\bar{m}^2}\end{aligned}$$

where $\Delta^2\omega$ is the dispersion , $\langle\omega^2\rangle - \langle\omega\rangle^2$, in ω and $\Delta^2\vec{k}$ is similarly defined. One thus obtains, in the limit of negligible dispersions, the time-like constraint of special relativity, simply becaues $m_0^2c^2\delta\tau^2$ is positive. One could just as easily obtain the space-like constraint for tachyons with $m_0^2 \rightarrow -m_0^2$. This analysis is another example of how the properties of τ are analogous to those of proper time.

It appears here that the as yet unspecified constant $\bar{m}$ should be identified as m_0, the expectation value of the mass. If this is done, then in the non-quantum limit of zero dispersions Eq. (4.10) reduces to the classical definition of proper-time interval, but in terms of expectation values.

Here, then, one sees that the FSF can be used to derive results that are familiar from special relativity. Furthermore, Eq. (4.7) represents the fact that the rest mass has been elevated in the FSF from simply a specified constant to an observable. An examination of Eq. (4.2) shows that Ψ is a superposition of states, each of which corresponds to a particular combination of $\vec{k}$ and ω. Thus one obtains the reasonable result that measurements of the mass of the relativistic particle are not sharply defined, but have a distribution that depends on the probabilistic weight of each pure state, namely $|A(\vec{k},\omega)|^2$. As an example let us consider the minimum wave packet representation of the free particle.

The expansion coefficients for the minimum wave packet are

$$A(\vec{k},\omega) = \int_{-\infty}^{\infty} \left\{ \left[\exp\left(-i k^{\mu} x_{\mu}\right) \right] \prod_{\mu=0}^{3} N_{\mu} \Psi_{\mu} \right\} d^4x \qquad (4.11)$$

where $\{N_\mu\}$ are normalization constants and $\{\Psi_\mu\}$ represent the initial wave components at $\tau = 0$ for the minimum wave packet; these are given by

$$\Psi_\mu = \left[2\pi (\Delta x^\mu)^2\right]^{-1/2} \cdot \exp\left\{ \frac{-(x^\mu - \langle x_0^\mu \rangle)^2}{4(\Delta x^\mu)^2} - i \langle k_{\mu 0} \rangle x^\mu \right\} . \qquad (4.12)$$

Here Δx^{μ} is the uncertainty in x^{μ}, and $\langle x_0^{\mu}\rangle$ and $\langle k_0^{\mu}\rangle$ represent the average position and momentum of the particle at the initial instant $\tau = 0$. The minimum wave packet is then constructed by substituting Eq. (4.11) into Eq. (4.2) and evaluating the integral. The result is

$$\Psi_{min}(\vec{x}, ct, \tau) = \prod_{\mu=0}^{3} \frac{N_{\mu}}{\sqrt{2\pi}} \left[\frac{\pi}{(\Delta x^{\mu})^2 + i\hbar\tau g_{\mu\mu}/2\bar{m}}\right]^{1/2} \tag{4.13}$$

$$\cdot \exp\left\{ i\langle k^{0}_{\mu}\rangle x^{\mu} - \frac{i\hbar\tau}{2\bar{m}}\langle k_0^{\mu}\rangle\langle k_{\mu 0}\rangle - \frac{(x^{\mu} - \langle x_0^{\mu}\rangle - \hbar\langle k_0^{\mu}\rangle\tau/\bar{m})^2}{4[(\Delta x^{\mu})^2 + i\hbar\tau g_{\mu\mu}/2\bar{m}]}\right\}$$

where $g_{\mu\mu}$ is given by

$$g_{00} = 1 = -g_{11} = -g_{22} = -g_{33} \ . \tag{4.14}$$

Before proceeding to the physically interesting points regarding Ψ_{min}, let us first emphasize two important mathematical points. First, the repeated indicies in Eqs. (4.12) and (4.13) do <u>not</u> imply summation. Second, take special note of the appearance of $g_{\mu\mu}$ in the expression for the minimum wave packet. If $g_{\mu\mu}$ did not appear in Eq. (4.13) as it does, then Ψ_{min} would not be a solution of Eq. (2.19) for the free particle case. With these remarks out of the way, let us now consider four physically interesting points.

First, notice that the averages $\langle\vec{x}\rangle$ and $\langle ct\rangle$ are $\langle\vec{x}_0\rangle + (\hbar\langle\vec{k}_0\rangle/\bar{m})\tau$ and $c\langle t_0\rangle + (\hbar\langle\omega_0\rangle/\bar{m}c)\tau$ respectively. These are the expected results.

Second, by taking the absolute square of $A(\vec{k},\omega)$ one obtains the probability distribution in the momentum-energy representation. The result is a Gaussian distribution which indicates that the wave packet is formed as a superposition of states that separately correspond to a particular mass, i.e. a particular combination of $\vec{k}$ and ω'. This is also expected.

Third, the absolute square of Ψ_{min} gives the probability distribution--Gaussian--in space <u>and</u> time. From this joint distribution a marginal probability distribution on the time domain is constructed representing the probability of observing the particle somewhere in space during a specified interval of time, i.e. $\rho(\vec{x},ct|\tau)$ is integrated over all space to yield $\bar{\rho}(ct|\tau)$. Whenever the marginal probability distribution is zero the particle cannot be observed <u>anywhere</u> in space, i.e. the particle effectively does not exist when $\bar{\rho}$ is zero. This capability, not present in conventional theories, is necessary for describing unstable particles in a single-particle formalsim.

Finally it is of interest to note that the wave packet solution, Ψ_{min}, is not Lorentz invariant. This is a result of the choice of the minimum wave packet as the initial value. Since $\prod_{\mu=0}^{3}\Phi_\mu$ is not Lorentz invariant, it is clear that the form of the initial value changes from one Lorentz frame to another. The consequence is that Ψ_{min} has a form that depends on the particular Lorentz frame. Although Ψ_{min} is not a relativistically proper wave packet, it does illustrate the concept of superposition of mass states.

V. SCATTERING FROM A STEP POTENTIAL

It is important to observe that the solutions of the usual KG equation have not been changed by going to a four-space formalism although the use of those solutions has changed. In addition, the definition of spatial probability flux as $\rho V^j (j=1,2,3)$ remains unchanged. If one recalls that scattering calculations require only the continuity of spatial probability flux, and do not require the use of normalized solutions, then it is evident that the usual KG theory can be used to compute scattering cross sections. To do so one must assume that the solution of Eq. (3.1) is stationary with respect to τ and represents a single mass state. In a rigorous treatment, however, these assumptions do not, in general, hold. It is then necessary to represent an incident free particle by a space-time wave packet which is a superposition of mass states, just as in NRQM an incident free particle is represented by a wave packet which is a superposition of energy states. The formal development of such a theory has promise as a fertile area for future research. For the purposes of this paper, however, it will be sufficient to consider only the simple example of a RSP scattering from a step potential.

As pointed out in Section I.B, an especially peculiar feature of conventional theories is the prediction that a RSP incident on a step potential of sufficient strength will be reflected by the barrier with a reflection coefficient that exceeds unity. This result is a direct consequence of identifying ej^0/c as the charge density. Even though total charge is conserved, the prediction that more particles will be reflected than were incident is a surprising consequence which has no experimental justification. This is a serious flaw of conventional theories that, as will be shown, does not arise in the FSF.

The four-vector potential for this problem is

$$A^0(x) = \begin{cases} 0 \,, & x \leq 0 \\ \alpha \,, & x > 0 \end{cases} \; ; \tag{5.1}$$

$$\vec{A}\,(\vec{x}, ct) = 0.$$

The time component, $A^0(x)$, is sketched in Figure 1.

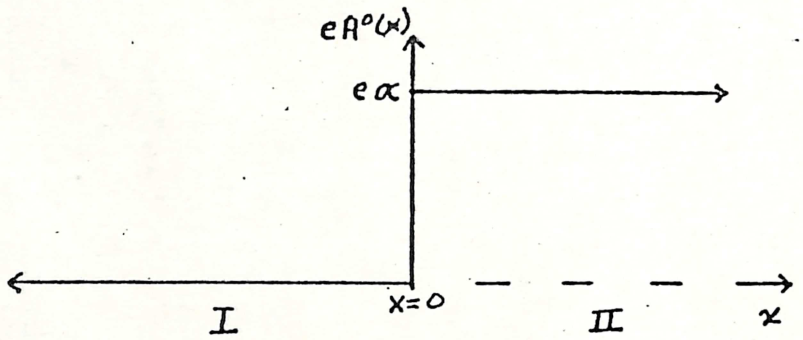

Figure 1: The Step Potential

It will be assumed throughout this calculation that a spinless tardyon is incident from the left of Figure 1 with energy ω_1 and momentum k_1, where ω_1 and k_1 are both real and positive. The boundary conditions to be satisfied are that the wavefunction and its first derivative with respect to x must be continuous across the boundary at x = 0.

The solutions of the equations

$$(2m\,i\hbar)\frac{\partial \psi_I}{\partial \tau} = g_I \psi_I = -\hbar^2\left[\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right]\psi_I \tag{5.2}$$

and

$$(2m\,i\hbar)\frac{\partial \psi_{II}}{\partial \tau} = g_{II}\psi_{II} = \hbar^2\frac{\partial^2}{\partial x^2}\psi_{II} + \left[\frac{\hbar}{ic}\frac{\partial}{\partial t} - \frac{e\alpha}{c}\right]^2\psi_{II} \tag{5.3}$$

are the wavefunctions for Regions I and II respectively.

In Region I the solution ψ_I is

$$\psi_I = \left[a_1 e^{-ik_1 x} + b_1 e^{ik_1 x}\right] e^{i\omega_1 t}\, e^{-ig_I\tau/2m\hbar} \tag{5.4}$$

where a_1 and b_1 are the coefficients of the incident and reflected plane wave solutions respectively. These identifications are established in Appendix B. The eigenvalue relation in Region I is

$$g_I \equiv m^2c^2 = \hbar^2\left(\frac{\omega_1^2}{c^2} - k_1^2\right) \geq 0 \tag{5.5}$$

where the inequality is valid for incident tardyons and the real quantity m is defined by Eq. (5.5). Since ω_1 and k_1 are assumed known, so also is the observed rest mass, m, of the particle.

A description of the situation in Region II is a little more involved than that given above for

Region I. The solution of Eq. (5.3) is

$$\Psi_{II} = \left[a_2 e^{-ik_2x} + b_2 e^{ik_2x}\right] e^{i\omega_2 t} e^{-ig_{II}\tau/2m\hbar}. \qquad (5.6)$$

To assure that the wavefunction and its first x-derivative are continuous at x = 0 for all values of t and τ one must have

$$\omega_1 = \omega_2 \qquad (5.7)$$

and

$$g_I = g_{II} \qquad (5.8)$$

respectively. The eigenvalue relation for Region II can now be written as

$$\hbar^2 k_2^2 = \left[\frac{\hbar\omega_1}{c} - \frac{e\alpha}{c}\right]^2 - m^2c^2 \qquad (5.9)$$

where k_2 may be real or imaginary. The four possible cases, the appropriate spatial solutions, and the reflection and transmission coefficients for each case, found in the same manner as that of NRQM[35], are listed in Table 3. The quantities ω_1, k_1, k_2, m^2c^2, and $e\alpha$ are all taken to be real and positive in Table 3. The coefficient b_2 is zero in Cases 1 and 3 because no particles are incident on the barrier from $x = +\infty$. For Cases 2 and 4 the quantity k_2 of Eq. (5.6) is positive imaginary thus the coefficient of the term $\exp(|k_2|x)$ must be zero because the wavefunction must be finite for all values of x. Are the results of Table 3 physically realistic?

In Table 3 it is evident that the reflection coefficient for each case does not exceed unity and that the sum of the reflection and transmission coefficients for each case is unity. These are desired results. All of the results for Cases 1 and 4 are easy to accept since these particular cases correspond to the familiar results of NRQM. The details of Cases 2 and 3 deserve further attention.

It is readily shown that Case 2 is physically realistic. First it is observed that $\hbar\omega_1 \geq mc^2$ because of Eq. (5.5). The eigenvalue condition for Case 2 can be written as

$$|e\alpha| \geq \hbar\omega_1 - mc^2 \geq 0 \qquad (5.10)$$

Recalling that the kinetic energy of the particle in Region I is $\hbar\omega_1 - mc^2$, it is clear that Eq. (5.10) asserts that the barrrier height exceeds the kinetic energy of the incident particle and, hence, that reflection at the barrier is expected. Thus the results of Case 2 are realistic.

Now consider Case 3. The smallest value of $|e\alpha|$ for which the conditions of Case 3 are satisfied is $2mc^2$. This is a very large value--on the order of 280 MeV for a charged pion--and is not yet experimentally accessible; consequently one cannot say with certainty whether or not Case 3 is physically realistic. Such a determination must await further technological advances.

From these considerations it is clear that three of the above four cases are physically realistic. There is not sufficient information available for a conclusion to be drawn regarding the fourth case, Case 3. It is hoped that experimentalists will strive to answer this question in the future.

The primary advantage of the FSF with regard to the scattering problem considered here is the elimination of reflection coefficients that exceed unity. This achievement further justifies acceptance of the FSF as the proper quantum mechanical description of RSP.

Table 3: Scattering From a Step Potential

Case	Conditions[a]	Spatial Solution	Reflection Coefficient R	Transmission Coefficient T	R+T=1?
1	$\hbar\omega_1 > e\alpha$ $\left[\frac{\hbar\omega_1}{c} - \frac{e\alpha}{c}\right]^2 \geq m^2c^2$	$a_2 e^{-ik_2x}$	$\left[\frac{k_1-k_2}{k_1+k_2}\right]^2$	$\frac{2k_1k_2}{(k_1+k_2)^2}$	YES
2	$\hbar\omega_1 > e\alpha$ $\left[\frac{\hbar\omega_1}{c} - \frac{e\alpha}{c}\right]^2 < m^2c^2$	$b_2 e^{-k_2x}$	1	0	Yes
3	$\hbar\omega_1 < e\alpha$ $\left[\frac{\hbar\omega_1}{c} - \frac{e\alpha}{c}\right]^2 \geq m^2c^2$	$a_2 e^{-ik_2x}$	$\left[\frac{k_1-k_2}{k_1+k_2}\right]^2$	$\frac{2k_1k_2}{(k_1+k_2)^2}$	Yes
4	$\hbar\omega_1 < e\alpha$ $\left[\frac{\hbar\omega_1}{c} - \frac{e\alpha}{c}\right]^2 < m^2c^2$	$b_2 e^{-k_2x}$	1	0	Yes

a. All of the quantities $_1$, e , m^2c^2, k_1, and k_2 are real and positive here.

VI. A TEST OF THE FOUR-SPACE FORMALISM: THE RELATIVISTIC SPINLESS PARTICLE BOUND BY A COULOMB POTENTIAL

The preceeding four chapters have resolved all but one of the difficulties discussed in Section I.B. The remaining difficulty arises because conventional theories define the expectation value of a function f as

$$\langle f\rangle_{con} = \left[\int_{-\infty}^{\infty} f\, j^{o}/c\, d^{3}x\right] \Big/ \int_{-\infty}^{\infty} j^{o}/c\, d^{3}x \qquad (6.1)$$

where j^{0}/c is given by

$$\frac{j^{o}}{c} = \frac{-i\hbar}{2mc^{2}}\left[\psi_{q}^{*}\frac{\partial\psi_{q}}{\partial t} - \psi_{q}\frac{\partial\psi_{q}^{*}}{\partial t}\right] - \frac{eA^{o}}{mc^{2}}\psi_{q}^{*}\psi_{q} \qquad (6.2)$$

with ψ_q a solution of the eigenvalue problem

$$q\,\psi_{q} = p^{\mu}p_{\mu}\,\psi_{q}\,. \qquad (6.3)$$

It will be shown in this chapter that $\langle f\rangle_{con}$ does not reduce, in the non-relativistic limit, to the value calculated using NRQM; whereas the procedures of the FSF do yield, in the proper limit, the value obtained using NRQM. Before proceeding further, let us first ascertain the region in which one should expect the expectation value defined in the FSF, $\langle\,\rangle_{FSF}$, to agree with that defined in NRQM, $\langle\,\rangle_{NRQM}$.

Observe that the joint probability density $\rho(\vec{x},ct|\tau)$ can always be written as the product of a marginal, $\bar{\rho}(t|\tau)$, and a conditional, $\rho_c(\vec{x}|ct,\tau)$, probability density:

$$\rho(\vec{x},ct|\tau) = \bar{\rho}(t|\tau)\,\rho_c(\vec{x}|ct,\tau). \qquad (6.4)$$

Now $\langle g\rangle_{FSF}$ is given by

$$\langle g\rangle_{FSF} = \int \bar{\rho}(t|\tau)\left\{\int g(\vec{x},ct)\,\rho_c(\vec{x}|ct,\tau)\,d^3x\right\} d(ct) \qquad (6.5)$$

where $g(\vec{x},ct)$ is, at present, unspecified. Equation (6.5) reduces to the three-space definition of expectation value only for those cases in which either the function g or else $\bar{\rho}(t|\tau)$ is independent of t. This is a mathematical constraint. To completely define the region in which $\langle\rangle_{FSF}$ should agree with $\langle\rangle_{NRQM}$ one must also impose the physical constraint that $\hbar\omega \sim m_0c^2$ where m_0 is the rest mass of the particle. This same physical requirement must also be imposed on $\langle\rangle_{con}$ before it can be compared with $\langle\rangle_{NRQM}$.

A special case which satisfies all of the above conditions is that in which one takes the expectation value of a function of the spatial coordinates, $f(\vec{x})$, and the time dependence of Ψ_q is $(\exp(i\omega t))/\sqrt{2T}$ where $-T<t<+T$ in the limit as $T\rightarrow\infty$. The resulting expectation values are

$$\langle f\rangle_{con} = \frac{\int_{-\infty}^{\infty} \psi_q^*\psi_q\,(\hbar\omega - eA^0)\,f(\vec{x})\,d^3x}{\int_{-\infty}^{\infty} \psi_q^*\psi_q\,(\hbar\omega - eA^0)\,d^3x} \qquad (6.6)$$

and

$$\langle f\rangle_{FSF} = \frac{\lim_{T\to\infty} \int_{-T}^{T}\int_{-\infty}^{\infty} f(\vec{x})\, \psi_g^{*}\psi_g \, d^3x \, d(ct)}{\lim_{T\to\infty} \int_{-T}^{T}\int_{-\infty}^{\infty} \psi_g^{*}\psi_g \, d^3x \, d(ct)} \tag{6.7}$$

where box normalization has been imposed in the time domain. Equation (6.7) can be written in the equivalent form

$$\langle f\rangle_{FSF} = \frac{\int_{-\infty}^{\infty} f(\vec{x})\, \psi_g^{*}\psi_g \, d^3x}{\int_{-\infty}^{\infty} \psi_g^{*}\psi_g \, d^3x} . \tag{6.8}$$

The important difference between $\langle f\rangle_{con}$ and $\langle f\rangle_{FSF}$ is due to the eA^0 term in $\langle f\rangle_{con}$. If either A^0 or f is independent of the spatial coordinates, then Eqs. (6.6) and (6.8) agree; generally they do not.

It is well known that the KG equation reduces[35] to the Schrödinger equation in the non-relativistic limit, although this violates both Lorentz invariance and the gauge is altered. Therefore the solutions in the non-relativistic limit are just the solutions of the Schrödinger equation and it is easy to see that Eq. (6.8) becomes the usual non-relativistic definition of the expectation value. It is also clear that $\langle f\rangle_{con}$ does not, in general, reduce to the non-relativistic limit because of the term of order $eA^0/\hbar\omega$. The magnitude of this discrepancy will be illustrated for the case in which A^0 is the Coulomb potential:

$$eA^0 = -\frac{Ze^2}{r} . \tag{6.9}$$

The solutions of the KG equation for the Coulomb potential are well known. To facilitate evaluation of the integrals it will be assumed that $\gamma^2 \approx$ (Z/137) is very small compared to $(\ell + \frac{1}{2})^2$ where ℓ is a positive integer; one can then use the recurrence relations and orthonormality condition of the associated Laguerre functions. Using these solutions to determine the expectation value of the radius r gives

$$\langle r \rangle_{FSF} = \frac{2n}{\alpha}\left[1 + \frac{1}{2}\left(1 - \frac{\ell(\ell+1)}{n^2}\right)\right] \tag{6.10}$$

and

$$\langle r \rangle_{con} = \frac{\left\{ \frac{4n^2 \hbar\omega}{\alpha}\left[1 + \frac{1}{2}\left(1 - \frac{\ell(\ell+1)}{n^2}\right)\right] + 2neZ \right\}}{2n\hbar\omega - \alpha e^2 Z} \tag{6.11}$$

where n is a non-zero positive integer and

$$\alpha = \frac{2\omega}{c}\,\frac{Z}{m}\left[\frac{e}{\hbar c}\right]. \tag{6.12}$$

Dividing $\langle r \rangle_{con}$ by $\langle r \rangle_{FSF}$ yields

$$\frac{\langle r \rangle_{con}}{\langle r \rangle_{FSF}} = \frac{n^2\delta + Z^2}{\delta\left[n^2 + Z^2\beta^2\right]} \approx 1 + \frac{Z^2}{n^2\delta} \gtrsim 1 + \frac{Z^2}{n^2\delta} \tag{6.13}$$

where

$$\delta \equiv 1 + \frac{1}{2}\left(1 - \frac{\ell(\ell+1)}{n^2}\right), \quad \beta = \frac{e^2}{\hbar c} \sim \frac{1}{137}. \tag{6.14}$$

The last step of Eq. (6.14) follows because $Z^2\beta^2$ has been assumed negligible relative to a positive integer. The magnitude of the difference between $\langle r \rangle_{con}$ and $\langle r \rangle_{FSF}$ is now easily obtained. Suppose a π^- particle is bound by the Coulomb potential due to a Helium nucleus. If the π^- is in the 2P state then $\langle r \rangle_{con}$ is 80% larger than $\langle r \rangle_{FSF}$. This substantial difference* persists in the non-relativistic limit.

One can readily check the non-relativistic limit of $\langle r \rangle_{FSF}$ by first rewriting it as

$$\langle r \rangle_{FSF} = \frac{n^2}{Z} \frac{\hbar^2}{\left[\frac{\hbar\omega}{c^2}\right] e^2} \delta \, . \tag{6.15}$$

In the non-relativistic limit $\hbar\omega \sim m_0 c^2$ and Eq. (6.15) becomes

$$\langle r \rangle_{FSF} \rightarrow \frac{n^2}{Z} \frac{\hbar^2}{m_0 e^2} \delta \tag{6.16}$$

which is precisely the result calculated using the non-relativistic Schrödinger theory. The non-relativistic limit of $\langle r \rangle_{con}$ is

$$\langle r \rangle_{con} \cong \frac{n^2}{Z} \frac{\hbar^2}{m_0 e^2} \delta \left[1 + \frac{Z^2}{\delta n} \right] \tag{6.17}$$

which differs significantly from the expected result. The above comparison clearly shows that the four-space formalism properly reduces to the non-relativistic limit for such stationary states but the conventional theories do not.

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* For a $\pi^- - \pi^+$ system $\langle r \rangle_{con}$ is 20% larger than $\langle r \rangle_{FSF}$ for the 2P state.

VII. CONCLUSIONS

The four-space formulation presented here exhibits a number of features which favor its acceptance as the proper quantum mechanical theory to be used when describing relativistic spinless particles.

First, the FSF <u>preserves the useful</u> features of conventional theories, i.e. the solutions of the usual KG equation are retained* and the usual procedure for calculating cross-sections from scattering theory can be employed.

Second, the FSF <u>removes an inadequacy</u> of conventional theories. In particular, the concept of "negative probability density" is replaced by the Born interpretation.

Third, <u>gaps</u> in conventional theories <u>are filled</u> by the FSF. These gaps are as follows:

i) Conventional theories cannot consistently define a Hermitian Hamiltonian, and hence orthonormality relations except for the free particle case.

ii) Conventional theories fail to provide a

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* The eigenvalues have been reinterpreted, however.

correspondence to non-quantum relativistic mechanics although such a correspondence should exist. The FSF does provide such a correspondence.

iii) Conventional theories do not interpret j^0/c for neutral particles and their antiparticles in a mathematically non-trivial manner. The FSF does provide a proper framework for such particles.

iv) Existing single-particle theories cannot consistently describe particle decay. The FSF does.

Fourth, the FSF provides a resolution of the Klein paradox which, it is hoped, will be experimentally tested in the future.

Fifth, the FSF corrects an error of conventional theories. Specifically, the non-relativistic limit of expectation values defined by conventional theories does not agree with the expectation values of NRQM in the region where agreement is expected. The expectation values defined by the FSF do agree, within the proper range of applicability, with those of NRQM.

A significant aspect of the approach taken here to formulate the FSF is that it places probabilistic concepts as the basis of quantum theory. This approach offers avenues for further development; in particular the topological interpretation of the Heisenberg Uncertainty Principle developed for the non-relativistic theory[25] then applies to this relativistic theory.

Though further development of the FSF is required before a firm conclusion can be drawn, it seems, in the light of the features exhibited in this paper, that this formalism does represent a consistent relativistic quantum mechanics for spinless particles. It is suggested that the four-space formalism should properly replace the conventional Klein-Gordon formalisms.

APPENDIX A: NOTATION

The metric $g_{\mu\nu}$ is given by

$$\{g_{\mu\nu}\} \equiv \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \tag{1}$$

The space-time coordinates (ct, x, y, z) are denoted by the contravariant four-vector

$$\{x^\mu\} \equiv (ct, x, y, z) = (x^0, x^1, x^2, x^3), \tag{2}$$

and the space-time covariant four-vector is

$$\{x_\nu\} = \{g_{\nu\mu} x^\mu\} = (x_0, x_1, x_2, x_3) = (ct, -\vec{x}). \tag{3}$$

The four-momentum in momentum space is

$$\{p^\mu\} = \left(\frac{E}{c}, p_x, p_y, p_z\right). \tag{4}$$

In k-space p^μ is given by

$$\{p^\mu\} = \hbar\left(\frac{\omega}{c}, k_x, k_y, k_z\right) \equiv \{\hbar k^\mu\}, \tag{5}$$

and in the coordinate representation the four-momentum operator is

$$\{p^\mu\} = \{i\hbar\, \partial_\mu\} \equiv \left(\frac{i\hbar}{c}\frac{\partial}{\partial t}, -i\hbar\nabla\right) \tag{6}$$

where

$$\partial_\mu \equiv \frac{\partial}{\partial x_\mu} . \tag{7}$$

The covariant form of the four-momentum operator is

$$\{p_\mu\} = \{i\hbar\partial^\mu\} = i\hbar\left(\frac{1}{c}\frac{\partial}{\partial t}, \vec{\nabla}\right) \tag{8}$$

where

$$\partial^\mu \equiv \frac{\partial}{\partial x^\mu} . \tag{9}$$

Lastly the four-vector potential is

$$\{A^\mu\} = (\Phi, \vec{A}) = \{g^{\mu\nu} A_\nu\} \tag{10}$$

where Φ is the real scalar potential and $\vec{A}$ is the real vector potential. The Einstein summation convention is invoked unless otherwise noted.

APPENDIX B. DIRECTION OF PARTICLE PROPAGATION FOR THE CASE OF SCATTERING FROM A STEP POTENTIAL

Recall that

$$\rho V^{\mu} = \frac{-i\hbar}{2\bar{m}}\left[\psi^{*}\frac{\partial\psi}{\partial x_{\mu}} - \psi\frac{\partial\psi^{*}}{\partial x_{\mu}}\right] - \frac{eA^{\mu}}{\bar{m}c}\psi^{*}\psi, \tag{11}$$

and

$$\begin{cases} \text{Region I:} & (A^{0}, A^{1}) = (0,0) \\ \text{Region II:} & (A^{0}, A^{1}) = (\alpha, 0) \,. \end{cases} \tag{12}$$

For the t and x components one has

$$\rho V^{0} = \frac{-i\hbar}{2\bar{m}c}\left[\psi^{*}\frac{\partial\psi}{\partial t} - \psi\frac{\partial\psi^{*}}{\partial t}\right] - \frac{eA^{0}}{\bar{m}c}\psi^{*}\psi \tag{13}$$

and

$$\rho V^{1} = \frac{i\hbar}{2\bar{m}}\left[\psi^{*}\frac{\partial\psi}{\partial x} - \psi\frac{\partial\psi^{*}}{\partial x}\right] \tag{14}$$

respectively. One can now determine the propagation direction for a given plane wave solution in a specified region. These results are tabulated in Table 4.

Table 4: Propagation Direction
of Plane Wave Solutions

Region[a]	Ψ	V^0	V^1	Propagation Direction
I	$e^{i\omega t}$	$\frac{\hbar\omega}{\bar{m}c}$	—	Forward in t
	$e^{-i\omega t}$	$-\frac{\hbar\omega}{\bar{m}c}$	—	Backward in t
	e^{ikx}	—	$-\frac{\hbar k}{\bar{m}}$	Backward in x
	e^{-ikx}	—	$\frac{\hbar k}{\bar{m}}$	Forward in x
II	$e^{i\omega t}$	$\frac{\hbar\omega - e\alpha}{\bar{m}c}$	—	Forward in t if $\hbar\omega > e\alpha$ Backward in t if $\hbar\omega < e\alpha$ Stationary in t if $\hbar\omega = e\alpha$
	$e^{-i\omega t}$	$\frac{-\hbar\omega - e\alpha}{\bar{m}c}$	—	Backward in t
	e^{ikx}	—	$-\frac{\hbar k}{\bar{m}}$	Backward in x
	e^{-ikx}	—	$\frac{\hbar k}{\bar{m}}$	Forward in x

a. The quantities ω, k and $e\alpha$ are all real and positive.

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