Second Quantization of the Square-Root Klein-Gordon Operator.

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ABSTRACT

The square-root Klein-Gordon operator, $\sqrt{m^2 - \nabla^2}$, is a non-local operator with a natural scale inversely proportional to the mass (the Compton wavelength). There is no fundamental reason to exclude negative energy states from a "square-root" propagation law. We find several possible Hamiltonians associated with $\sqrt{m^2 - \nabla^2}$ which include both positive and negative energy plane wave states. It is possible to satisfy the equations of motion with commutators or anticommutators. For the scalar case, only the canonical commutation rules yield a stable vacuum. We investigate microscopic causality for the commutator of the Hamiltonian density. We find that despite the non-local dependence of the energy density on the field operators, the commutators of the physical observables vanish for space-like separations. Hence, Pauli's result [1] can be extended to the non-local case. Pauli explicitly excluded $\sqrt{m^2 - \nabla^2}$ because this operator acts non-locally in the coordinate space. The Mandelstam representation offers the possibility of avoiding the difficulties inherent in minimal coupling (Lorentz invariance and gauge-invariance). We also compute the propagators for the scattering problem and investigate the solutions of the square-root equation in the Aharonov-Bohm problem.

1. Introduction

There is much interest in applications of the square-root Klein-Gordon operator, $\sqrt{m^2 - \nabla^2}$, to problems in quantum mechanics. The square-root operator appears in applications of the Bethe-Salpeter equation to bound states of quarks [2] and again in the general problem of binding in very strong fields [3]. The problem of the relativistic string (bosonic strings) also involves a square-root operator [4] and therefore this problem is especially relevant to modern particle theory in a way that is different than the original context. A long misunderstood point relates to the negative energy states. There is no fundamental reason to exclude such states and we suggest that it is perfectly natural to take the negative square root along with the positive square root. Our purpose will be to indicate how this can be consistently done in quantum field theory. The result in the scalar case will reduce to the standard second quantized Klein-Gordon Hamiltonian in the non-interacting case, but will be a distinctly new theory in the presence of interactions.

Our motivation for studying this operator is that it is the natural extension of the classical energy function into quantum mechanics. The impact made by the non-local behavior of $\sqrt{m^2 - \nabla^2}$ on causality has been investigated [5] for wave packets in ordinary quantum mechanics and has led to a theorem regarding localization. We are particularly interested in causality questions that arise from the application of the procedure of second quantization.

In section 2 we review the physical picture based on de Broglie waves and discuss some of the mathematical tools that can be used to define the action of $\sqrt{m^2 - \nabla^2}$ on functions. Section 3 develops the second quantization of the equation associated with $\sqrt{m^2 - \nabla^2}$ and examines the commutation relations of the observable quantities. In section 4 we investigate the commutation rules for the

Klein-Gordon Hamiltonian density operator and the expectation value for this commutator for states in Fock-space. We see that for an arbitrary state in Fock-space the expectation value of the commutator does not vanish at space-like separation. In section 5 we consider the requirement of a stable vacuum and normal ordering. Section 6 derives the propagators for the 1-, 2-, and 3-dimensional problem in an infinite domain for both the time-dependent and stationary scattering problem. Section 7 reviews minimal coupling and the difficulty with using minimal coupling in the square-root operator. In section 8 it is shown that the Mandelstam representation of interactions is Lorentz-invariant and gauge invariant in the presence of the square-root operator and provides a counter example to the conclusion of [12]. The Mandelstam representation of interactions therefore has deep and fundamental significance and has distinct advantages over minimal coupling in that it can be extended to non-local Hamiltonians in a Lorentz invariant manner. Section 9 considers the scattering problem for the Aharonov-Bohm effect for the square-root equation in the presence of a finite magnetic flux confined to the z-axis. Section 10 extends the scalar square-root equation to the zero-mass spin-1/2 case. Section 11 briefly considers restricting $\sqrt{m^2 - \nabla^2}$ to finite domains and the implications for the function spaces that $\sqrt{m^2 - \nabla^2}$ acts upon. Section 12 presents a proof that the second quantized square-root Hamiltonian does not reduce to the second quantized Klein-Gordon Hamiltonian in the presence of interactions. Interactions are introduced by applying the Mandelstam procedure. Section 13 presents a summary and conclusions of the implications of $\sqrt{m^2 - \nabla^2}$ on microscopic causality, minimal coupling, and interactions.

2. Relativistic de Broglie Waves

Let us consider a scalar wave function describing a relativistic particle propagating through space. The form of the wave function for a particle of mass m, traveling along the x-direction is given by

$$\psi = Ae^{-i(\omega t - k \cdot x)}, \tag{1}$$

where $\omega = \sqrt{m^2 + k^2}$ is the energy, A is the amplitude, and k is the momentum. We note that the phase velocity is given by

$$v_{\text{phase}} = \frac{dx}{dt} = \frac{\omega}{k} > 1, \tag{2}$$

and hence the phase velocity is always greater than the velocity of light. For freely propagating waves the phase is not observable and only modulations in the amplitude are observable. However, we can get modulations only by superimposing waves with different frequencies and this leads us to consider wave packets. It is well known that the wave packets formed by such superpositions have amplitudes whose centers propagate at the group velocity. This is given by

$$v_{\text{group}} = \frac{d\omega}{dk} = \frac{k}{\sqrt{m^2 + k^2}} < 1. \tag{3}$$

The concept of causality that applies to the above simple example is that the significant information propagates with a velocity less than the speed of light. This satisfies the idea of classical causality. There has been no attempt to incorporate the quantum mechanical effects associated with the uncertainty principle. It is of some interest to consider what other types of causality constraints are consistent with the uncertainty principle of quantum mechanics [6], but we will not go into this question any further.

Let us examine the equation of motion that the above wave function satisfies. For a pure positive frequency we have

$$i\frac{\partial\psi}{\partial t} = \omega_k\psi = \sqrt{m^2+k^2}\psi, \tag{4}$$

and for a superposition of frequencies the above equation holds for each frequency component. We can express the equation of motion for the general wave function as

$$i\frac{\partial\psi}{\partial t} = \sqrt{m^2-\nabla^2}\;\psi. \tag{5}$$

If we set the mass to zero in Eq. (5) and interpret ψ as a vector-valued function, then we arrive at a non-local representation of the photon wave equation [7]. In this case the operator on the Right-Hand-Side (RHS) of Eq. (5) is related to the "half-Laplacian" operator which is useful in the theory of elliptic self-adjoint operators [8]. In addition "half derivatives" also have a long history [9].

There are several techniques available to define the square-root Klein-Gordon operator seen on the RHS of Eq. (5). We can use path integrals [10], semi-groups of operators (functional calculus) [11], the operator calculus [12], and also pseudodifferential operators [13].

If one considers eigenfunctions of the modified Helmholtz operator

$$(m^2-\nabla^2)f_\lambda(x) = \lambda f(x), \tag{6}$$

then it follows [14] from the theory of functional analysis that

$$\sqrt{m^2-\nabla^2}\;f_\lambda(x) = \sqrt{\lambda}f(x). \tag{7}$$

Hence if one uses a complete set of eigenfunctions one can use the set to define the action of $\sqrt{m^2-\nabla^2}$ on any function by projecting an arbitrary function onto the eigenfunctions and summing over all eigenfunctions. Such an approach can be illustrated explicitly with Fourier transforms, since the exponential functions involved are the prototype eigenfunctions for most operators. Fourier transforms are the basis of the theory of pseudodifferential operators.

From the point of view of relativistic de Broglie waves, the most straightforward way to define the square-root is in terms of pseudodifferential operators via the Fourier transform. One obtains an integral representation of an operator as follows. Consider an operator $p(x, D)$ where $D_i = -i\partial/\partial x^i$. The action of $p(x, D)$ on a function ψ is given in terms of Fourier transforms as

$$p(x, D)\psi(x) = \frac{1}{(2\pi)^n} \int\limits_{R^n} \int\limits_{K^n} e^{ik\cdot x} p(x, k) e^{-ik\cdot y} \, d^n k \psi(y) \, d^n y, \tag{8}$$

(R^n refers to n-dimensional Euclidean space and K^n refers to the corresponding Fourier transform space). In Eq. (8), $p(x, k)$ is known as the *symbol* of $p(x, D)$. Symbols provide a very useful way to work with operators. We can use a multiplicative calculus [15] instead of an operator calculus (i.e., operator inversion is represented by symbol division). Symbols essentially give a representation of the operator on phase space. This gives us a kernel function for the integral representation defined by

$$K(x, y) = \frac{1}{(2\pi)^n} \int\limits_{K^n} e^{ik\cdot x} p(x, k) e^{-ik\cdot y} \, d^n k, \tag{9}$$

and therefore

$$p(x, D)\psi(x) = \int\limits_{R^n} K(x, y)\psi(y) \, d^n y. \tag{10}$$

The operator, $\sqrt{m^2 - \nabla^2}$, is a fractional power of the modified Helmholtz operator $(m^2 - \nabla^2)$. H. Weyl [16] grasped the significance of using integral kernels to represent the square-root operator and considered the relativistic problem. Weyl's idea of defining the operator corresponding to a symbol [17] is very similar to the concept of modern pseudodifferential operators. Unfortunately Weyl did not develop a complete theory. The square-root operator approach to relativistic quantum mechanics was subsequently abandoned and new approaches were tried leading to the Klein-Gordon equation and the Dirac equation.

Pseudodifferential operators give us a representation of $\sqrt{m^2 - \nabla^2}$ acting on a function ψ as follows

$$\begin{aligned}
\sqrt{m^2 - \nabla^2}\,\psi &= \int\limits_{R^3} \frac{1}{(2\pi)^3} \int\limits_{K^3} e^{ik\cdot(x-y)} \sqrt{m^2 + k^2}\, d^3k\, \psi(y)\, d^3y, \\
&= (m^2 - \nabla^2) \int\limits_{R^3} \frac{1}{(2\pi)^3} \int\limits_{K^3} \frac{e^{ik\cdot(x-y)}}{\sqrt{m^2 + k^2}}\, d^3k\, \psi(y)\, d^3y, \qquad (11) \\
&= (m^2 - \nabla^2) \int\limits_{R^3} \frac{m}{2\pi^2} \frac{K_1(m|x-y|)}{|x-y|}\, \psi(y)\, d^3y.
\end{aligned}$$

The kernel function in Eq. (11) has a singularity on the diagonal $x = y$ and is a smooth function off the diagonal. The singularity on the diagonal is characteristic of pseudodifferential operators and is what makes them similar to local differential operators. It is called the *pseudolocal property* [18]. In fact if the kernel were a finite linear combination of the derivatives of the δ-function then the operator $p(x, D)$ would be a a differential operator. In this case we would be considering a purely local operator–a polynomial in the derivative operator.

3. Second Quantization of the Square-Root Klein-Gordon Equation

In order to proceed with the Quantum Field Theory (QFT), we note that Eq. (5) can be derived from the Lagrangian density

$$\mathcal{L}(x) = \psi^* \left[i\frac{\partial}{\partial t} - \sqrt{m^2 - \nabla^2} \right] \psi. \tag{12}$$

Variation with respect to ψ^* produces Eq. (5). The Lagrangian in Eq. (12) is very similar to what one would obtain by second quantization of the Schrödinger equation [19] but it has a non-local Lagrangian density. Variation with respect to ψ results in the complex conjugate equation

$$-i\frac{\partial \psi^*}{\partial t} = \sqrt{m^2 - \nabla^2}\, \psi^*. \tag{13}$$

The canonically conjugate field variable to ψ is given by

$$\pi = \frac{\partial \mathcal{L}}{\partial \dot{\psi}} = i\psi^*. \tag{14}$$

We can express the Lagrangian density in field-operator language as

$$\mathcal{L} = \psi^\dagger \left[i\frac{\partial}{\partial t} - \sqrt{m^2 - \nabla^2} \right] \psi, \tag{15}$$

where we replace ψ^* by $\psi^\dagger$ to signify the transition from functions to field operators. The Hamiltonian density operator associated with the above Lagrangian is given by

$$\begin{aligned} \mathcal{H} &= \pi\dot{\psi} - \mathcal{L} \\ &= \psi^\dagger \sqrt{m^2 - \nabla^2}\, \psi. \end{aligned} \tag{16}$$

In the above representation the Hamiltonian density is not symmetrized with respect to ψ and $\psi^\dagger$. It is possible to extend the Hamiltonian of Eq. (16) by symmetry considerations. For example one might consider the symmetric or antisymmetric combinations

$$\mathcal{H}_+ = \frac{1}{2}\left[\psi^\dagger\sqrt{m^2-\nabla^2}\,\psi + \psi\sqrt{m^2-\nabla^2}\,\psi^\dagger\right], \tag{17}$$

$$\mathcal{H}_- = \frac{1}{2}\left[\psi^\dagger\sqrt{m^2-\nabla^2}\,\psi - \psi\sqrt{m^2-\nabla^2}\,\psi^\dagger\right]. \tag{18}$$

In order to investigate the canonical equations of motion we define anticommutators and commutators

$$[\psi(x), \psi^\dagger(x')]_\pm \equiv \psi(x)\psi^\dagger(x') \pm \psi^\dagger(x')\psi(x), \tag{19}$$

where the + sign gives the anticommutator and the − sign gives the commutator. From Eq. (19) we can solve for the products of the fields

$$\begin{aligned} \psi(x)\psi^\dagger(x') &= \mp\psi^\dagger(x')\psi(x) + [\psi(x), \psi^\dagger(x')]_\pm, \\ \psi^\dagger(x')\psi(x) &= \mp\psi(x)\psi^\dagger(x') \pm [\psi(x), \psi^\dagger(x')]_\pm. \end{aligned} \tag{20}$$

Commutation relations can be imposed at equal time and then extrapolated to arbitrary time differences using the time development of the field operators. Consider the equal-time commutation relations

$$\begin{aligned} &[\psi(x), \psi(x')]_\pm = [\psi^\dagger(x), \psi^\dagger(x')]_\pm = 0, \text{ and} \\ &[\psi(x), \psi^\dagger(x')]_\pm = \delta^3(x-x'). \end{aligned} \tag{21}$$

In Eq. (21) we can opt for either the + sign or the − sign in the commutator and then we must check to see if the canonical equations and microscopic causality conditions are consistent with that choice. We will examine the Hamiltonian densities of Eq. (16), Eq. (17), and Eq. (18) to see which commutation relations are consistent with the canonical equations of motion. Using the first line of Eq. (21) the following list of equal-time commutation relations can be obtained

$$
\begin{aligned}
[\psi(x),\psi^{\dagger}(y)\sqrt{m^2-\nabla_y^2}\psi(y)] &= [\psi(x),\psi^{\dagger}(y)]_{\pm}\sqrt{m^2-\nabla_y^2}\psi(y), \\
[\psi(x),\psi(y)\sqrt{m^2-\nabla_y^2}\psi^{\dagger}(y)] &= \mp\psi(y)\sqrt{m^2-\nabla_y^2}[\psi(x),\psi^{\dagger}(y)]_{\pm}, \\
[\psi^{\dagger}(x),\psi^{\dagger}(y)\sqrt{m^2-\nabla_y^2}\psi(y)] &= -\psi^{\dagger}(y)\sqrt{m^2-\nabla_y^2}[\psi(y),\psi^{\dagger}(x)]_{\pm}, \\
[\psi^{\dagger}(x),\psi(y)\sqrt{m^2-\nabla_y^2}\psi^{\dagger}(y)] &= \pm[\psi(y),\psi^{\dagger}(x)]_{\pm}\sqrt{m^2-\nabla_y^2}\psi^{\dagger}(y).
\end{aligned}
\tag{22}
$$

The canonical equations of motion have the form

$$
\begin{aligned}
i\frac{\partial\psi}{\partial t} &= [\psi, H]\,, \\
i\frac{\partial\psi^{\dagger}}{\partial t} &= \left[\psi^{\dagger}, H\right],
\end{aligned}
\tag{23}
$$

where $H(t) = \int \mathcal{H}(y,t)\,d^3y$. We can insert Eq. (16), Eq. (17), or Eq. (18) into Eq. (23) and simplify the result by making use of Eq. (22) and the following adjointness property [20]

$$
\int f(x)[\sqrt{m^2-\nabla^2}\; g(x)]\,d^3x = \int [\sqrt{m^2-\nabla^2}\; f(x)]g(x)\,d^3x. \tag{24}
$$

If the canonical equations, Eq. (23), are to be consistent with Eq. (5) and Eq. (13), then we obtain restrictions on the commutation relations between the field operators ψ and $\psi^{\dagger}$. If we consider the Hamiltonian density of Eq. (16), then using the commutation relations we obtain the result that

$$
\begin{aligned}
[\psi(x), H] &= \int [\psi(x), \psi^\dagger(y)]_\pm \sqrt{m^2 - \nabla_y^2}\psi(y)\, d^3y, \\
&= \int \delta^3(x-y)\sqrt{m^2 - \nabla_y^2}\psi(y)\, d^3y, \\
&= \sqrt{m^2 - \nabla_x^2}\psi(x).
\end{aligned}
\tag{25}
$$

We also obtain

$$
\begin{aligned}
[\psi^\dagger(x), H] &= -\int \psi^\dagger(y)\sqrt{m^2 - \nabla_y^2}[\psi(y), \psi^\dagger(x)]_\pm\, d^3y, \\
&= -\int \psi^\dagger(y)\sqrt{m^2 - \nabla_y^2}\delta^3(x-y)\, d^3y, \\
&= -\sqrt{m^2 - \nabla_x^2}\psi^\dagger(x).
\end{aligned}
\tag{26}
$$

Hence we conclude that the canonical equations of motion associated with the Hamiltonian density of Eq. (16) are consistent with Eq. (5) and Eq. (13) independent of whether anticommutation or commutation relations are used in the second quantization procedure. Let us denote the operator in the second term in Eq. (17) or Eq. (18) as $\mathcal{H}_1$ (i.e., $\mathcal{H}_1 \equiv \psi\sqrt{m^2 - \nabla^2}\,\psi^\dagger$). The commutation relations for $\mathcal{H}_1$ are

$$
\begin{aligned}
[\psi(x), \mathcal{H}_1] &= \mp\int \psi(y)\sqrt{m^2 - \nabla_y^2}[\psi(x), \psi^\dagger(y)]_\pm\, d^3y, \\
&= \mp\int \psi(y)\sqrt{m^2 - \nabla_y^2}\delta^3(x-y)\, d^3y, \\
&= \mp\sqrt{m^2 - \nabla_x^2}\psi(x).
\end{aligned}
\tag{27}
$$

and

$$
\begin{aligned}
[\psi^\dagger(x), \mathcal{H}_1] &= \pm \int [\psi(y), \psi^\dagger(x)]_\pm \sqrt{m^2 - \nabla_y^2}\psi^\dagger(y)\, d^3y, \\
&= \pm \int \delta^3(x-y)\sqrt{m^2 - \nabla_y^2}\psi^\dagger(y)\, d^3y, \\
&= \pm \sqrt{m^2 - \nabla_x^2}\psi^\dagger(x).
\end{aligned} \tag{28}
$$

In view of the sign dependence in the above equations we see that the Hamiltonian density Eq. (17) is consistent with Eq. (5) and Eq. (13) only if commutation relations are used in the second quantization. Also we note Eq. (18) is consistent with Eq. (5) and Eq. (13) only if anticommutation relations define the second quantization. We do not attempt at this point to decide between the different Hamiltonians so far considered. We simply note that it is possible to introduce Bosonic or Fermionic statistics by symmetrization. Also the Hamiltonian density in Eq. (16) is consistent with the basic equations of motion regardless of the type of statistics of the field operators.

Recently a treatment of second quantization of the square-root Klein-Gordon equation was published [21] which considered only the canonical commutation rules and positive energy states. It is important to consider commutation rules as well as anti-commutation rules and investigate the consequences of normal ordering as will be shown below. Furthermore, the restriction to positive energy states in [21] makes *microscopic* causality impossible and one can derive only *macroscopic* causality. In addition [21] implies that minimal coupling can be used to describe interactions. Minimal coupling in the presence of the square-root operator violates Lorentz invariance [12] and hence one must look for another method to incorporate interactions.

Let us explore the most general plane-wave states associated with the above canonical equations of motion. We ask: *Where are the negative square-root solutions?* There is no fundamental reason for excluding negative energy states (negative frequency plane waves) from the theory. Therefore, we expand the field operator into plane-wave states that contain positive and negative frequencies

$$\phi(x,t) = \frac{1}{\sqrt{2(2\pi)^3}} \int\limits_{K^3} \left[a(k)\, e^{i(k\cdot x - \omega t)} + b^\dagger(k)\, e^{-i(k\cdot x - \omega t)} \right] d^3k. \tag{29}$$

Several things should be noted about the field operator in Eq. (29). First, it is not Hermitian because we are dealing with a complex field as opposed to a real field. *Second, the normalization is different from that of the field associated with the Klein-Gordon equation.* Specifically, notice that there is no factor of $\omega_k = \sqrt{m^2 + k^2}$ multiplying the $(2\pi)^3$. Similarly we have

$$\phi^\dagger(x,t) = \frac{1}{\sqrt{2(2\pi)^3}} \int\limits_{K^3} \left[a^\dagger(k)\, e^{-i(k\cdot x - \omega t)} + b(k)\, e^{i(k\cdot x - \omega t)} \right] d^3k. \tag{30}$$

Because Eq. (29) is a superposition of positive and negative frequencies care must be taken to construct Hamiltonian densities that are consistent with the equations of motion for both the positive and negative frequencies. Consider a field operator, $\chi(x,t)$, related to $\phi(x,t)$ and given by

$$\chi(x,t) = \frac{1}{\sqrt{2(2\pi)^3}} \int\limits_{K^3} \left[a(k)\, e^{i(k\cdot x - \omega t)} - b^\dagger(k)\, e^{-i(k\cdot x - \omega t)} \right] d^3k. \tag{31}$$

χ and ϕ form a doublet [22] of fields given by

$$\psi = \begin{bmatrix} \phi \\ \chi \end{bmatrix}. \tag{32}$$

The equations of motion are given by

$$i\beta\frac{\partial\psi}{\partial t} = \sqrt{m^2 - \nabla^2}\,\psi, \tag{33}$$

where

$$\beta = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \tag{34}$$

We can think of the above as a two-component formulation of the theory with each component being composed of mixtures of positive and negative frequencies. For purely positive frequencies the field has the form

$$\psi(x,t) = \begin{bmatrix} \psi^+(x,t) \\ \psi^+(x,t) \end{bmatrix} \tag{35}$$

and for purely negative frequency states the field has the form

$$\psi(x,t) = \begin{bmatrix} \psi^-(x,t) \\ -\psi^-(x,t) \end{bmatrix}. \tag{36}$$

The above equations of motion can be derived from the Lagrangian

$$\mathcal{L} = i\psi^\dagger\beta\frac{\partial\psi}{\partial t} - \psi^\dagger\sqrt{m^2 - \nabla^2}\,\psi, \tag{37}$$

with corresponding Hamiltonian given by

$$\mathcal{H} = \psi^\dagger\sqrt{m^2 - \nabla^2}\,\psi. \tag{38}$$

The above two-component formulation of the square-root equation theory can be reduced to the Klein-Gordon theory in the free-field case by making the following transformation on the field operators

$$\hat{\phi} = (m^2 - \nabla^2)^{-1/4}\phi,$$
$$\hat{\chi} = (m^2 - \nabla^2)^{1/4}\chi. \tag{39}$$

With this transformation the Hamiltonian in Eq. (38) becomes

$$\mathcal{H} = \hat{\chi}^\dagger \hat{\chi} + \hat{\phi}^\dagger (m^2 - \nabla^2)\hat{\phi}, \tag{40}$$

which is clearly equivalent to the standard Klein-Gordon Hamiltonian density after performing an integration-by-parts and ignoring the surface terms at infinity

$$\mathcal{H} = \hat{\chi}^\dagger \hat{\chi} + \nabla\hat{\phi}^\dagger \cdot \nabla\hat{\phi} + m^2 \hat{\phi}^\dagger \hat{\phi}. \tag{41}$$

Commutation relations between field operators can be related to commutation relations between the expansion coefficients $a(k), a^\dagger(k)$ and $b(k), b^\dagger(k)$. We shall start with equal-time commutation relations

$$\begin{aligned}
&[\chi(x), \chi(x')]_\pm = [\chi^\dagger(x), \chi^\dagger(x')]_\pm = 0,\\
&[\phi(x), \phi(x')]_\pm = [\phi^\dagger(x), \phi^\dagger(x')]_\pm = 0,\\
&[\chi(x), \chi^\dagger(x')]_\pm = 0,\\
&[\phi(x), \phi^\dagger(x')]_\pm = 0, \text{ and}\\
&[\chi(x), \phi^\dagger(x')]_\pm = [\phi(x), \chi^\dagger(x')]_\pm = \delta^3(x - x').
\end{aligned} \tag{42}$$

Inserting the expansions for $\psi(x,t)$ we obtain

$$\begin{aligned}
[a(k), a(k')]_\pm &= [a^\dagger(k), a^\dagger(k')]_\pm = 0, \\
[b(k), b(k')]_\pm &= [b^\dagger(k), b^\dagger(k')]_\pm = 0, \\
[a(k), b(k')]_\pm &= [a(k), b^\dagger(k')]_\pm = 0, \\
[a^\dagger(k), b(k')]_\pm &= [a^\dagger(k), b^\dagger(k')]_\pm = 0, \\
[a(k), a^\dagger(k')]_\pm &= \delta^3(k-k'), \quad \text{and} \\
[b(k), b^\dagger(k')]_\pm &= \delta^3(k-k').
\end{aligned} \tag{43}$$

Using the above equal-time anticommutation/commutation rules we can calculate the values for arbitrary space-like or time-like separations. For notational purposes let $kx = k \cdot x - \omega t$. We obtain

$$\begin{aligned}
[\chi(x), \phi^\dagger(x')]_\pm = \frac{1}{2(2\pi)^3} \int \Big[[a(k), a^\dagger(k')]_\pm \, e^{i(kx - k'x')} \quad - \\
[b^\dagger(k), b(k')]_\pm \, e^{-i(kx-k'x')} \Big] \, d^3k \, d^3k',
\end{aligned} \tag{44}$$

which reduces to

$$[\chi(x), \phi^\dagger(x')]_\pm = \frac{1}{2(2\pi)^3} \int \left[e^{ik(x-x')} \mp e^{-ik(x-x')} \right] d^3k. \tag{45}$$

Except for the relative sign, observe that the second term in the above integral is just the complex conjugate of the first term. We examine the first term and integrate over the azimuthal and polar angles to obtain

$$\frac{1}{(2\pi)^2} \left(-\frac{1}{r} \frac{\partial}{\partial r} \right) \int_0^\infty e^{-it\sqrt{m^2+k^2}} \, \cos(kr) \, dk. \tag{46}$$

The integral in the above formula [23] can be evaluated to obtain

$$\int_0^\infty \exp^{-it\sqrt{m^2+k^2}} \cos(kr)\, dk = \lim_{\epsilon \to 0} m(it+\epsilon) \frac{K_1\left(m\sqrt{r^2+(it+\epsilon)^2}\right)}{\sqrt{r^2+(it+\epsilon)^2}}, \tag{47}$$

where $K_1(x)$ is a modified Bessel function.

As one can see, for space-like separations one can take the limit in the above formula and derive the result that the RHS is purely imaginary for space-like separations. This means that the commutator $[\chi(x), \phi^\dagger(x')]_\pm$, evaluated at space-like separations, is the sum of a purely imaginary function and minus or plus it's complex conjugate. Consequently the two terms on the RHS of Eq. (45) cancel out entirely for space-like separations *using commutation rules* whereas the anti-commutator does not vanish. For time-like separation we can analytically continue the result to imaginary arguments. Let us factor out $-i$ and keep in mind that we have to take the $\epsilon \to 0$ limit of

$$im(it+\epsilon) \frac{K_1\left(-im\sqrt{-(it+\epsilon)^2 - r^2}\right)}{\sqrt{-(it+\epsilon)^2 - r^2}}. \tag{48}$$

By using the relationship $K_\nu(x) = \frac{\pi}{2} i^{\nu+1} H_\nu^{(1)}(ix)$, we can write the above result as

$$\frac{\pi t m}{2\sqrt{t^2-r^2}} H_1^{(1)}(m\sqrt{t^2-r^2}). \tag{49}$$

Now the $H_\nu^{(1)}$ are Hankel functions and contain real and imaginary combinations of ordinary Bessel functions and Neumann functions. We have $H_\nu^{(1)}(x) = J_\nu(x) + iN_\nu(x)$, where the ordinary Bessel function and Neumann function are real functions of real arguments in this case (i.e., the only imaginary quantity left is the

i that multiplies the Neumann function). This allows us to finish the calculation of the commutator of the field operators at time-like separations by noticing that again the imaginary part of the first term will cancel the imaginary part of the second term in the commutator and we are left with

$$[\chi(x), \phi^\dagger(x')]_- = -\frac{tm}{4\pi}\frac{1}{r}\frac{\partial}{\partial r}\frac{J_1(m\sqrt{t^2-r^2})}{\sqrt{t^2-r^2}}. \tag{50}$$

For completeness we consider a broader class of integrals that appear often in questions regarding microscopic causality

$$\begin{aligned} I_n^{\pm}(x) &= \frac{1}{2(2\pi)^3}\int \omega_k^n \left[e^{-ikx} \pm e^{ikx}\right] d^3k, \\ &= \frac{1}{4\pi^2}\left(i\frac{\partial}{\partial t}\right)^n \int \left[e^{-ikx} \pm (-1)^n e^{ikx}\right] d^3k. \end{aligned} \tag{51}$$

When the two exponential functions in the integral have the same sign then the integral vanishes outside the lightcone. When there is a relative sign difference between the two exponential functions then their respective contributions do not cancel outside the lightcone. Therefore, for $I_n^+(x)$, the even powers of ω_k vanish when x is space-like and the odd powers do not. For $I_n^-(x)$, the odd powers of ω_k vanish when x is space-like and the even powers do not.

4. Commutators for the Hamiltonian Density Functions

As a first consideration we explore the real Klein-Gordon Hamiltonian density

$$H = \frac{1}{2} \int\limits_{R^3} \left[\pi^2 + (\vec{\nabla}\psi)^2 + m^2\psi^2 \right] d^3x, \tag{52}$$

where $\psi(x)$ is the field operator and $\pi \equiv \nabla_t \psi$ is the canonically conjugate operator. Using the expansion of the field operators for the real Klein-Gordon field we obtain

$$\psi(x) = \frac{1}{\sqrt{2(2\pi)^3}} \int\limits_{K^3} \frac{1}{\sqrt{\omega_k}} \left[a(k)e^{-ikx} + a^\dagger(k)e^{ikx} \right] d^3k, \tag{53}$$

where $\omega_k = \sqrt{m^2 + k^2}$ and $a(k)$ and $a^\dagger(k)$ are expansion operators that satisfy the following commutation relations

$$\begin{aligned} [a(k), a^\dagger(k')] &= \delta^3(k - k'), \\ [a(k), a(k')] &= [a^\dagger(k), a^\dagger(k')] = 0. \end{aligned} \tag{54}$$

Let us follow Friedrichs in the evaluation of the Hamiltonian density. We have the following relations [24]

$$\begin{aligned} \int f(x)\sqrt{m^2 - \nabla^2}\, g(x)\, d^3x &= \int g(x)\sqrt{m^2 - \nabla^2}\, f(x)\, d^3x, \\ \int (\sqrt{m^2 - \nabla^2}\, f(x))(\sqrt{m^2 - \nabla^2}\, f(x))\, d^3x &= \int f(x)(m^2 - \nabla^2) f(x)\, d^3x, \\ -\int f(x)\nabla^2 f(x))\, d^3x &= \int (\vec{\nabla} f(x))^2\, d^3x. \end{aligned} \tag{55}$$

Using the relations in Eq. (55) we can rewrite the Klein-Gordon Hamiltonian density operator as

$$
\begin{aligned}
&\int \left[\pi^2 + (\vec{\nabla}\psi)^2 + m^2\psi^2\right] d^3x = \\
&\int \Big[\{\sqrt{m^2-\nabla^2}\,\psi(x,t) - i\pi(x,t)\}\{\sqrt{m^2-\nabla^2}\,\psi(x,t) + i\pi(x,t)\} \\
&+ i[(\sqrt{m^2-\nabla^2}\,\psi)\pi - \pi\sqrt{m^2-\nabla^2}\,\psi]\Big]\, d^3x.
\end{aligned}
\tag{56}
$$

The last term on the RHS above has the following form based on the commutation relations

$$
\begin{aligned}
i[(\sqrt{m^2-\nabla^2}\,\psi)\pi - \pi\sqrt{m^2-\nabla^2}\,\psi] &= -\sqrt{m^2-\nabla^2}\ \delta^3(x-x), \\
&= -\sqrt{m^2-\nabla^2}\ \delta(0).
\end{aligned}
\tag{57}
$$

Therefore this term is an infinite c-number and can be associated with the so-called "zero-point energy." Since it is a c-number we need not concern ourselves with it in the calculation of the commutator for the Klein-Gordon Hamiltonian at different points. The remaining operator on the RHS of Eq. (56) is finite [25]. Let us now compute the commutator of the Klein-Gordon Hamiltonian at different space-time points and explore the meaning of the commutator for different states in Fock-space. We first define some axillary fields that can be used to further reduce the Hamiltonian [26]

$$
A^{\pm} = \frac{1}{\sqrt{2}}\left[(m^2-\nabla^2)^{1/4}\psi \mp i(m^2-\nabla^2)^{-1/4}\pi\right].
\tag{58}
$$

In terms of the operators that define $\psi(x)$ we have

$$
\begin{aligned}
A^{+}(x) &= \frac{1}{\sqrt{(2\pi)^3}}\int\limits_{K^3} a(k)e^{-ikx}\, d^3k, \\
A^{-}(x) &= \frac{1}{\sqrt{(2\pi)^3}}\int\limits_{K^3} a^{\dagger}(k)e^{ikx}\, d^3k.
\end{aligned}
\tag{59}
$$

The equal-time commutation relations for the $A^{\pm}(x)$ operators are

$$\begin{aligned}
\big[A^{+}(x), A^{-}(x')\big]_{-} &= \delta^{3}(x - x'), \\
\big[A^{+}(x), A^{+}(x')\big]_{-} &= 0, \\
\big[A^{-}(x), A^{-}(x')\big]_{-} &= 0.
\end{aligned} \tag{60}$$

The finite operator part of the Klein-Gordon Hamiltonian can be expressed in terms of the $A^{\pm}$ as follows

$$\mathcal{H}(x) = A^{+}(x)\sqrt{m^{2} - \nabla^{2}}\, A^{-}(x). \tag{61}$$

We can calculate the commutator

$$\begin{aligned}
\big[\mathcal{H}(x), \mathcal{H}(x')\big] &= A^{+}(x)\sqrt{m^{2} - \nabla_{x}^{2}}A^{-}(x)A^{+}(x')\sqrt{m^{2} - \nabla_{x'}^{2}}A^{-}(x') \\
&\quad - A^{+}(x')\sqrt{m^{2} - \nabla_{x'}^{2}}A^{-}(x')A^{+}(x)\sqrt{m^{2} - \nabla_{x}^{2}}A^{-}(x).
\end{aligned} \tag{62}$$

Using the above commutation rules we can expand the RHS of Eq. (62) into

$$\begin{aligned}
&\big[\mathcal{H}(x), \mathcal{H}(x')\big] = \\
&A^{+}(x)\sqrt{m^{2} - \nabla_{x}^{2}}\Big[A^{+}(x')A^{-}(x) + [A^{-}(x), A^{+}(x')]_{-}\Big]\sqrt{m^{2} - \nabla_{x'}^{2}}A^{-}(x') \\
&-A^{+}(x')\sqrt{m^{2} - \nabla_{x'}^{2}}\Big[A^{+}(x)A^{-}(x') + [A^{-}(x), A^{+}(x')]_{-}\Big]\sqrt{m^{2} - \nabla_{x}^{2}}A^{-}(x).
\end{aligned} \tag{63}$$

Because

$$[A^{+}(x), A^{-}(x')]_{-} = \frac{1}{(2\pi)^{3}}\int e^{-ik(x-x')}d^{3}k, \tag{64}$$

we have

$$\sqrt{m^{2} - \nabla_{x}^{2}}[A^{-}(x), A^{+}(x')]_{-} = \sqrt{m^{2} - \nabla_{x'}^{2}}[A^{-}(x), A^{+}(x')]_{-}. \tag{65}$$

We can therefore factor out this c-number from the above product and cancel like operator terms by use of the commutation rules. We are left with

$$\begin{aligned}\left[\mathcal{H}(x),\mathcal{H}(x')\right] &= \sqrt{m^2-\nabla_x^2}[A^-(x),A^+(x')]_- \\ \times\Big[A^+(x)\sqrt{m^2-\nabla_{x'}^2}A^-(x') &- A^+(x')\sqrt{m^2-\nabla_x^2}A^-(x)\Big].\end{aligned} \tag{66}$$

Inserting the expansions for the $A^{\pm}(x)$ operators we are left with

$$\begin{aligned}\left[\mathcal{H}(x),\mathcal{H}(x')\right] &= \frac{1}{(2\pi)^3}\sqrt{m^2-\nabla_x^2}[A^-(x),A^+(x')]_- \\ \times\int\int\sqrt{m^2+k^2}\,\Big[a(k')a^\dagger(k)e^{i[kx'-k'x]} &- a(k')a^\dagger(k)e^{i[kx-k'x']}\Big]\,d^3k d^3k'.\end{aligned} \tag{67}$$

Now we consider the matrix elements of this operator for the diagonal elements of Fock-space (i.e., no transitions between initial and final states), $\Psi_i=\Psi_f=\Psi$. At this point we note that the operator product $a(k)a^\dagger(k')$ acts diagonally for identical initial and final states and is related to the number operator, $n_k=a^\dagger(k')a(k)$, in the occupation number representation for the Fock-space by the commutation rules. We have

$$\begin{aligned}a^\dagger(k)a(k') &= n_k\delta_{kk'}, \\ a(k)a^\dagger(k') &= (1+n_k)\delta_{kk'}.\end{aligned} \tag{68}$$

Hence

$$\begin{aligned}<\Psi|\left[\mathcal{H}(x),\mathcal{H}(x')\right]|\Psi> &= \frac{1}{(2\pi)^3}\sqrt{m^2-\nabla_x^2}[A^-(x),A^+(x')]_- \\ \times\left(i\frac{\partial}{\partial t}\right)\int(1+n_k)&\left[e^{-ik(x-x')}+e^{ik(x-x')}\right]\,d^3k.\end{aligned} \tag{69}$$

In the case of the vacuum state, $|\Psi>=|0>$, Eq. (62) would commute for space-like separation because we would have a time derivative of $I_0^+(x-x')$ in Eq. (69) (i.e., $n_k=0$ for the vacuum). However if n_k is non-zero then there would be only special cases that would have space-like commutativity of the Hamiltonian density (e.g., uniform density $n_k = 1$). Distributions that had only one state, $|\Psi >= |k >$, or thermal distributions

$$n_k = \frac{1}{e^{\beta\omega_k} - 1} = \sum_{n=1}^{\infty} e^{-n\beta\omega_k}, \tag{70}$$

where $\beta = 1/kT$ is the Boltzmann factor for thermal distributions, would not have the uniformity required to yield commutativity at space-like separation. Hence we conclude that the Klein-Gordon Hamiltonian density does not in general commute at space-like separation. Integration of the n_k term in Eq. (69) for a thermal distribution yields

$$\begin{aligned}\int n_k \left[e^{-ikx} + e^{ikx}\right] d^3k. &= \int \frac{1}{e^{\beta\omega_k} - 1} \left[e^{-ikx} + e^{ikx}\right] d^3k. \\ &= \sum_{n=1}^{\infty} \int e^{-n\beta\omega_k} \left[e^{-ikx} + e^{ikx}\right] d^3k. \\ &= \sum_{n=1}^{\infty} \frac{(n\beta + it)m}{\sqrt{r^2 + (n\beta + it)^2}} K_1 \left(m\sqrt{r^2 + (n\beta + it)^2}\right) + cc.\end{aligned} \tag{71}$$

Taking the case when $t = 0$ we see that Eq. (71) does not vanish for $r > 0$. Hence this example shows that the commutator of the Klein-Gordon Hamiltonian does not vanish in the presence of a thermal distribution at space-like intervals.

Let us now consider the case of the observables associated with the field operators for the Hamiltonians we have explored in section 3. We make the assumption that the observables will be in the form of bilinear combinations of the field operators and their Hermitian conjugates. For example an observable associated with the operator $\hat{O}_x$ of the first type is of the form $\psi^\dagger(x) O_x \psi(x)$. However, there could be more general forms of observables of the second type such as

$\hat{O}_x = \psi^\dagger(x) O_x \psi(x) \pm \psi(x) O_x \psi^\dagger(x)$. The commutators of the observables can be written either in terms of commutators or anticommutators of the field operators. The choice depends on what was imposed in the second quantization (i.e., the equal-time commutation relations). The commutator of an observable of the first type can be written as

$$\begin{aligned}[\hat{O}_x, \hat{O}_{x'}] =& O_x[\psi(x), \psi^\dagger(x')]_\pm \psi^\dagger(x) O_{x'} \psi(x') \\ & - O_{x'}[\psi(x'), \psi^\dagger(x)]_\pm \psi^\dagger(x') O_x \psi(x).\end{aligned} \tag{72}$$

For operators $\hat{O}$ that satisfy the following symmetry condition

$$O_x[\psi(x), \psi^\dagger(x')]_\pm = O_{x'}[\psi(x'), \psi^\dagger(x)]_\pm, \tag{73}$$

we can factor these c-numbers out of the operator products. Because of the anticommutation/commutation laws the above reduces in the special case of operators that satisfy Eq. (73) to

$$[\hat{O}_x, \hat{O}_{x'}] = O_x[\psi(x), \psi^\dagger(x')]_\pm \left(\psi^\dagger(x) O_{x'} \psi(x') - \psi^\dagger(x') O_x \psi(x) \right). \tag{74}$$

We conclude that any local Hermitian operator $\hat{O}$ will have an associated observable quantity that will satisfy microscopic causality because the commutators on the RHS of Eq. (74) vanish for space-like separations. In the case that $\hat{O}$ is a non-local operator a weaker statement can still be made in some cases. It should be mentioned that one would have a similar situation in ordinary QFT if one were to consider observables associated with non-local operators. This problem is not apparent in local QFT, because *all* the observables are assumed to be associated with local Hermitian operators. Suppose $\hat{O}$ is the operator $\sqrt{m^2 - \nabla^2}$. Then by the adjointness property, Eq. (24), we can consider the region that contributes to the double integral of the commutator over all of x and x'. In the case where $\hat{O}_x = \sqrt{m^2 - \nabla_x^2}$, we have for the first term on the RHS of Eq. (72)

$$\begin{aligned}\int \psi^\dagger(x)\overrightarrow{O_x}[\psi(x),\psi^\dagger(x')]_\pm \overrightarrow{O_{x'}}\psi(x')d^3xd^3x' = \\ \int \psi^\dagger(x)\overrightarrow{O_x}[\psi(x),\psi^\dagger(x')]_\pm \overleftarrow{O_{x'}}\psi(x')d^3xd^3x'.\end{aligned} \tag{75}$$

The arrows indicate the direction in which the operator is acting. Because of the form of the commutator function, we see that it is a function of $(x - x')$ and that the $\sqrt{m^2 - \nabla_x^2}$ operator acting on x in the commutator produces the same effect as $\sqrt{m^2 - \nabla_{x'}^2}$ acting on the x' argument. Hence the two operations of $\sqrt{m^2 - \nabla^2}$ combine and give the same result as the modified Helmholtz operator $(m^2 - \nabla^2)$ which is a local operator. Since the commutators vanish for space-like separations, the integrand will also vanish for space-like separations (the modified Helmholtz operator will not change this behavior). Therefore, only the time-like region (i.e., $(x - x')^2 > 0$) will contribute to the integral. This is also true for the second term on the RHS of Eq. (74). Hence we arrive at a weaker form of microscopic causality in the case of the observable quantity associated with the non-local operator $\sqrt{m^2 - \nabla^2}$, namely a case in which the integral of the commutator over both x and x' (spatial integrals) can be evaluated using only the time-like region.

Let us also consider an observable of the first type constructed from the Hamiltonian density associated with the general field operator in Eq. (29)

$$\tilde{\mathcal{H}}(x,t) = \{\phi^\dagger \sqrt{m^2 - \nabla^2}\,\phi + \chi^\dagger \sqrt{m^2 - \nabla^2}\,\chi\}. \tag{76}$$

In order to compute the commutator for the above operator function we define the following commutators

$$
\begin{aligned}
\mathcal{A}_1(x,x') &\equiv \left[\chi^\dagger(x)\sqrt{m^2-\nabla_x^2}\chi(x), \chi^\dagger(x')\sqrt{m^2-\nabla_{x'}^2}\chi(x')\right], \\
\mathcal{A}_2(x,x') &\equiv \left[\chi^\dagger(x)\sqrt{m^2-\nabla_x^2}\chi(x)], \phi^\dagger(x')\sqrt{m^2-\nabla_{x'}^2}\phi(x')\right], \\
\mathcal{A}_3(x,x') &\equiv \left[\phi^\dagger(x)\sqrt{m^2-\nabla_x^2}\phi(x), \chi^\dagger(x')\sqrt{m^2-\nabla_{x'}^2}\chi(x')\right], \\
\mathcal{A}_4(x,x') &\equiv \left[\phi^\dagger(x)\sqrt{m^2-\nabla_x^2}\phi(x), \phi^\dagger(x')\sqrt{m^2-\nabla_{x'}^2}\phi(x')\right].
\end{aligned} \tag{77}
$$

The commutator, $[\tilde{\mathcal{H}}(x), \tilde{\mathcal{H}}(x')]$ can be written as

$$
\tilde{\mathcal{H}}(x), \tilde{\mathcal{H}}(x')] = \mathcal{A}_1(x,x') + \mathcal{A}_2(x,x') + \mathcal{A}_3(x,x') + \mathcal{A}_4(x,x'). \tag{78}
$$

Evaluating these expressions we obtain (assuming commutation rules for the field operators as required by Eq. (45) and microscopic causality)

$$
\begin{aligned}
\mathcal{A}_1(x,x') &= I_1^-(x,x')\left[\chi^\dagger(x)\sqrt{m^2-\nabla_{x'}^2}\chi(x') + \chi^\dagger(x')\sqrt{m^2-\nabla_x^2}\chi(x)\right], \\
\mathcal{A}_2(x,x') &= I_1^+(x,x')\left[\chi^\dagger(x)\sqrt{m^2-\nabla_{x'}^2}\phi(x') - \phi^\dagger(x')\sqrt{m^2-\nabla_x^2}\chi(x)\right], \\
\mathcal{A}_3(x,x') &= I_1^+(x,x')\left[\phi^\dagger(x)\sqrt{m^2-\nabla_{x'}^2}\chi(x') - \chi^\dagger(x')\sqrt{m^2-\nabla_x^2}\phi(x)\right], \\
\mathcal{A}_4(x,x') &= I_1^-(x,x')\left[\phi^\dagger(x)\sqrt{m^2-\nabla_{x'}^2}\phi(x') + \phi^\dagger(x')\sqrt{m^2-\nabla_x^2}\phi(x)\right].
\end{aligned} \tag{79}
$$

Since $\mathcal{A}_1(x,x')$ and $\mathcal{A}_4(x,x')$ are both multiplied by $I_1^-(x,x')$, they both vanish for space-like $x-x'$. The sum of $\mathcal{A}_2(x,x')+\mathcal{A}_3(x,x')$ evaluated between Fock states $|\Psi>$ yields

$$
\begin{aligned}
&< \Psi|\left[\mathcal{A}_2(x,x') + \mathcal{A}_3(x,x')\right]||\Psi> = \\
&\quad \frac{1}{(2\pi)^3} I_1^+(x,x') \int \sqrt{m^2+k^2}(1+n_k+m_k)\left[e^{ik(x-x')} - e^{-ik(x-x')}\right] d^3k,
\end{aligned} \tag{80}
$$

which does not vanish outside the lightcone unless n_k and m_k are constants. Therefore as with the Klein-Gordon Hamiltonian density the above Hamiltonian density does not vanish unless special conditions hold true (i.e., $|\Psi >= |0>$, or n_k and m_k are constants).

5. Normal Ordering and Vacuum Stability

By using the adjointness property of $\sqrt{m^2 - \nabla^2}$ and also the commutation rules, we can derive

$$\begin{aligned} :\chi\sqrt{m^2-\nabla^2}\,\chi^\dagger: &= \mp :\chi^\dagger\sqrt{m^2-\nabla^2}\,\chi:, \\ :\phi\sqrt{m^2-\nabla^2}\,\phi^\dagger: &= \mp :\phi^\dagger\sqrt{m^2-\nabla^2}\,\phi:. \end{aligned} \tag{81}$$

Also

$$<\Psi| :\chi^\dagger\sqrt{m^2-\nabla^2}\,\chi: |\Psi>= \int \sqrt{m^2+k^2}\,[n_k \mp m_k]\; d^3k. \tag{82}$$

Hence $:\mathcal{H}_+:$ has non-zero expectation values when the fields are quantized with commutators and $:\mathcal{H}_-$ has non-zero expectation values when the field operators satisfy anti-commutation rules. However, only $:\mathcal{H}_+:$ has a stable vacuum (i.e., the vacuum is the minimum energy state). Hence we can rule out $:\mathcal{H}_-:$ on the physical grounds that it does not possess a stable vacuum and the associated field operators violate microscopic causality as seen in Eq. (45).

6. Propagation

6.1. Time-Dependent 1-Dimensional Propagator

Consider the equation

$$\left[i\beta\frac{\partial}{\partial t} - \sqrt{m^2 - \frac{\partial^2}{\partial x^2}}\right]\psi = 0. \tag{83}$$

The propagator for the above problem satisfies the following equation

$$\left[i\beta\frac{\partial}{\partial t} - \sqrt{m^2 - \frac{\partial^2}{\partial x^2}}\right]G(x - x') = \delta^2(x - x'). \tag{84}$$

Let us define the following operator (understood to act in the appropriate dimensional space for the problem at hand)

$$K_\pm = i\beta\frac{\partial}{\partial t} \mp \sqrt{m^2 - \nabla^2}\ . \tag{85}$$

We can multiply both sides of the above equation by

$$K_- = \left[i\beta\frac{\partial}{\partial t} + \sqrt{m^2 - \frac{\partial^2}{\partial x^2}}\right] \tag{86}$$

to obtain

$$\left[-\frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial x^2} - m^2\right]G(x - x') = K_-\delta^2(x - x'). \tag{87}$$

The operator on the Left-Hand-Side (LHS) is the Klein-Gordon operator and we can invert the operator using contour integration such that positive frequencies propagate forward in time and negative frequencies propagate backwards in time.

We obtain the following propagator for the 1-dimensional problem for positive frequencies

$$G_+(x-x') = -\frac{i}{2(2\pi)^2} K_- \begin{bmatrix} \frac{\pi}{2} H_0^{(2)}(m\sqrt{t^2-x^2}), & t>x \\ iK_0(m\sqrt{x^2-t^2}), & x>t \end{bmatrix} \tag{88}$$

For negative frequencies we obtain

$$G_-(x-x') = -\frac{i}{2(2\pi)^2} K_- \begin{bmatrix} \frac{\pi}{2} H_0^{(1)}(m\sqrt{t^2-x^2}), & t>x \\ -iK_0(m\sqrt{x^2-t^2}), & x>t \end{bmatrix} \tag{89}$$

6.2. Stationary 1-Dimensional Propagator

In the case of the steady-state scattering problem the time-independent propagator is the Fourier-Transform of the time-dependent propagator with respect to the time coordinate. It can also be calculated directly as follows

$$G_\omega(x) = \frac{1}{2\pi}\{\omega\beta + \sqrt{m^2-\nabla^2}\,\} \int_{-\infty}^{+\infty} \frac{dp}{\omega^2-p^2-m^2+i\epsilon}. \tag{90}$$

Performing the contour integration we obtain the following result for outgoing and incoming waves

$$\begin{aligned} G^o_{\pm\omega}(x) &= \frac{i}{2}(1\pm\beta)e^{ipx}, \\ G^i_{\pm\omega}(x) &= \frac{-i}{2}(1\pm\beta)e^{-ipx}. \end{aligned} \tag{91}$$

where o and i refer to outgoing and incoming respectively and the $\pm$ refers to the sign of the frequency ω. Also p is the relativistic momentum, $p = \sqrt{\omega^2 - m^2}$.

6.3. Time-Dependent 2-Dimensional Propagator

In this case we have the same relationship between the propagator for the square-root equation and the Klein-Gordon propagator as above. The time dependent propagator has the form

$$G_+(x-x') = \frac{-i}{2(2\pi)} K_- \begin{bmatrix} \sqrt{\dfrac{m\pi}{2(t^2-x^2)^{1/2}}} H^{(1)}_{-1/2}(m\sqrt{t^2-x^2}), & |t|>|x| \\ i\sqrt{\dfrac{2m}{\pi(t^2-x^2)^{1/2}}} K_{1/2}(m\sqrt{x^2-t^2}), & |x|>|t| \end{bmatrix} \tag{92}$$

For negative frequencies we obtain

$$G_-(x-x') = \frac{-i}{2(2\pi)} K_- \begin{bmatrix} \sqrt{\dfrac{m\pi}{2(t^2-x^2)^{1/2}}} H^{(2)}_{-1/2}(m\sqrt{t^2-x^2}), & |t|>|x| \\ -i\sqrt{\dfrac{2m}{\pi(t^2-x^2)^{1/2}}} K_{1/2}(m\sqrt{x^2-t^2}), & |x|>|t| \end{bmatrix} \tag{93}$$

6.4. Stationary 2-Dimensional Propagator

In the 2-dimensional case, we find the Greens' function for the stationary scattering problem to be

$$\begin{aligned} G^o_{\pm\omega}(\rho) &= -i(1\pm\beta)\sqrt{m^2+p^2}H^{(1)}_0(p\rho), \\ G^i_{\pm\omega}(\rho) &= i(1\pm\beta)\sqrt{m^2+p^2}H^{(2)}_0(p\rho). \end{aligned} \tag{94}$$

where o/i refer to outgoing/incoming cylindrical waves respectively, the $\pm$ refers to the sign of the frequency ω, and $p=\sqrt{\omega^2-m^2}$.

6.5. Time-Dependent 3-Dimensional Propagator

In the 3-dimensional case we simply note the method used to invert the Klein-Gordon operator and find

$$G(x) = K_{-} G_F(x), \tag{95}$$

where $G_F(x)$ is the Feynman propagator for the Klein-Gordon equation.

6.6. Stationary 3-Dimensional Propagator

The 3-dimensional Green's functions for the stationary scattering problem are given by

$$\begin{aligned} G^o_{\pm\omega}(r) &= \frac{1}{2(2\pi)^2}(1 \pm \beta)p\frac{e^{ipr}}{r}, \\ G^i_{\pm\omega}(r) &= \frac{1}{2(2\pi)^2}(1 \pm \beta)p\frac{e^{-ipr}}{r}. \end{aligned} \tag{96}$$

where o/i refer to outgoing/incoming spherical waves respectively, the $\pm$ refers to the sign of the frequency ω, and $p = \sqrt{\omega^2 - m^2}$.

7. The Inconsistency of the Operator $\sqrt{m^2 + (-i\nabla + e\vec{A}(x))^2}$

The assumption of minimal coupling is that interactions can be represented by modifying the derivative operator as follows

$$\partial_\mu \psi \to (\partial_\mu + ieA_\mu)\psi, \tag{97}$$

where A_μ is a four-vector potential representing the interactions and ψ represents the matter-field interacting with the four-vector potential. A_μ is further required to satisfy the local gauge transformation property

$$\psi' = \exp\{ie\theta(x)\}\psi,$$
$$A'_\mu = A_\mu - \partial_\mu\theta. \tag{98}$$

We show explicitly below that the above prescription breaks down in the general case of arbitrary functions $\theta(x)$ for the square-root Klein-Gordon operator. The only case where local gauge invariance works is when $\exp\{ie\theta(x)\}$ is an eigenfunction of ∇.

Let $\hat{h}(k) = \mathcal{F}[h(x)]$ represent the Fourier-transform operator

$$\hat{h}(k) = \mathcal{F}[h(x)] = \frac{1}{(2\pi)^{3/2}} \int e^{-ik\cdot x} h(x)\, d^3x. \tag{99}$$

Then the Fourier transform of the product of two functions is represented by the convolution theorem

$$\mathcal{F}[f(x)g(x)] = \frac{1}{(2\pi)^{3/2}} \int \hat{f}(k-\xi)\hat{g}(\xi) d^3\xi. \tag{99}$$

Using Fourier transforms we can represent the action of the square-root operator on ψ as follows

$$\begin{aligned} \sqrt{m^2 - \nabla^2}\ \psi(x,t) &= \frac{1}{(2\pi)^{3/2}} \int e^{ik\cdot x} \sqrt{m^2 + k^2}\ \hat{\psi}(k,t) d^3k, \\ &= \frac{1}{(2\pi)^3} \int e^{ik\cdot(x-y)} \sqrt{m^2 + k^2}\ \psi(y,t) d^3k d^3y. \end{aligned} \tag{100}$$

Consider multiplying ψ by a phase that is a function of space-time position

$$\psi'(x,t) = f(x,t)\psi(x,t), \tag{101}$$

where $f(x,t) = \exp\{ie\theta(x,t)\}$. By the convolution theorem of Fourier transforms we can represent the action of $\sqrt{m^2 - \nabla^2}$ on $\psi'(x,t)$ as follows

$$
\begin{aligned}
(2\pi)^3 \sqrt{m^2 - \nabla^2}\ \psi'(x,t) &= \int e^{ik\cdot x} \sqrt{m^2 + k^2}\ \int \hat{f}(k-\xi)\hat{\psi}(\xi,t) d^3\xi d^3k, \\
&= \int e^{ik\cdot x} \hat{f}(k) \int e^{i\xi\cdot x} \sqrt{m^2 + (k+\xi)^2}\ \hat{\psi}(\xi,t) d^3\xi d^3k, \\
&= (2\pi)^{3/2} \int e^{ik\cdot x} \hat{f}(k) \sqrt{m^2 + (\vec{k} - i\nabla)^2}\ \psi(x,t)\, d^3k.
\end{aligned}
\tag{102}
$$

The square-root operator therefore picks up a convolution over the wave-number in the expansion of the function $f(x)$. We operate with a shifted square-root operator on $\psi(x,t)$ and integrate the shifted operator weighted by $\hat{f}(k)$ (i.e., the operator is shifted by the Fourier wave-numbers of $f(x)$). This is essentially an eigenvalue expansion of $f(x)$ over the complete set of plane-waves. Notice that the gradient of $f(x)$ does not enter *directly* into the square-root operation.

This is very similar to the exponential-shift property of differential operators in the Heaviside operational calculus. In the Heaviside calculus a differential operator $P(D)$, (where is a polynomial in the derivative operator) enjoys the following property known as the exponential shift

$$
e^{-rx} P(D) e^{rx} f(x) = P(D+r) f(x), \tag{103}
$$

whereas the square-root operator obeys the following exponential-shift law

$$
e^{-ik\cdot x} \sqrt{m^2 - \nabla^2}\ e^{ik\cdot x} \psi(x) = \sqrt{m^2 + (\vec{k} - i\nabla)^2}\ \psi(x). \tag{104}
$$

We denote exponentially-shifted square-root operator as

$$
\sqrt{m^2 - \nabla^2}\ |_k = \sqrt{m^2 + (\vec{k} - i\nabla)^2}\,. \tag{105}
$$

Given the above arguments we have proven an inconsistency between the exponential-shift property of the square-root operator and the transformation properties of the four-potential required by gauge-invariance. Therefore in the case of gauge transformations on ψ of the form $f(x)\psi(x)$, where $f(x) = \exp\{ie\theta(x)\}$, we do not expect to see the gradient, $\nabla\theta(x)$, entering the square-root operator (unless in the trivial case $e\theta(x) = k \cdot x$).

Since this is the essential assumption of gauge-invariance for minimal coupling, we don't expect this method to hold true in the general case. The essential problem can be explicitly formulated by asking: Is minimal coupling consistent with gauge invariance given the shift property in the convolution formula of Eq. (102)? In order for this to be the case we insert the assumed form of minimal coupling in the square-root operator and perform the convolution required to represent the operation of $\sqrt{m^2 - \nabla^2}$ on $\exp\{ie\theta(x)\}\psi$. We obtain the following condition for the consistency of the operator, $\sqrt{m^2 + (-i\nabla + e\vec{A}(x))^2}$, constructed using the assumption of minimal coupling and local gauge-invariance

$$\begin{aligned}\frac{1}{(2\pi)^{3/2}} \int e^{ik\cdot x} \hat{f}(k) \sqrt{m^2 + (e\vec{A}'(x) + \vec{k} - i\nabla)^2}\, \psi(x,t)\, d^3k = \\ \exp\{ie\theta(x)\} \sqrt{m^2 + (e\vec{A}(x) - i\nabla)^2}\, \psi(x,t).\end{aligned} \tag{106}$$

The transformed four-vector potential, $A'_\mu(x,t)$, would therefore be required to transform as

$$\begin{aligned} A'_0(x,t) &= A_0(x,t) - \partial_t\theta(x,t), \\ \vec{A}'(x,t) &= \vec{A}(x,t) - \nabla\theta(x,t) = \vec{A}(x,t) - \vec{k}/e, \end{aligned} \tag{107}$$

which requires that the function $\theta(x,t)$ satisfy the relation

$$e\nabla\theta = \vec{k}. \tag{108}$$

This means that minimal coupling is not consistent with gauge invariance for the square-root Klein-Gordon equation except for the case of specific transformations functions satisfying

$$\nabla \exp\{ie\theta(x)\} = i\vec{k}\exp\{ie\theta(x)\}. \tag{109}$$

The above inconsistency between the exponential shift property of the square-root operator, the Fourier convolution theorem, and the requirement of local gauge invariance is severe and renders any application of minimal coupling to the square-root operator (except restricted by the above form) moot. Of course, the argument of this paper rests heavily on the assumption that the action of the square-root operator can be represented via Fourier transforms. Being that $\sqrt{m^2 - \nabla^2}$ is a fractional operator one must allow for the possibility that it is multi-valued ("half"-derivatives [27] are also multi-valued and disagreements existed between different operator definitions for the value of the half-derivative of unity, i.e., $\lim_{(m\to 0)} \frac{d^{1/2}x^m}{dx^{1/2}}$.) and therefore different representations of the operator acting on functions are possible. It is not beyond the realm of possibility that other representations of $\sqrt{m^2 - \nabla^2}$ would possibly allow minimal coupling. However, such definitions would fall outside of the realm of operators represented by Fourier transforms.

The non-local representation of minimal coupling [28] attempts to represent the gradient inside the square-root using the momentum-space representation

$$\begin{aligned} \vec{p} \rightarrow & [\vec{p} - e\vec{A}_t(q,p)], \quad \text{where} \\ \vec{A}_t(q,p) = & \int (d^3x)\, K(q,p,x)\vec{A}_{cl}(t,x), \quad A_0 = V, \\ & \int (d^3x)\, K(q,p,x) = 1. \end{aligned} \tag{110}$$

Exactly the same problem regarding gauge-invariance presents itself in the case of

Eq. (110). The exponential shift property does not bring $\nabla\theta$ inside the square-root and hence not inside the integral defining $\vec{A}_t(q,p)$. Therefore Eq. (110) does not admit gauge-invariance, since there is no way to transfer the addition of a gradient to $A_{cl}(t,x)$ from inside the square-root to a phase factor outside the square-root multiplying ψ.

We ask: Is there a generalization of the theory of interactions which will preserve gauge invariance in the presence of the square-root operator? One could consider a change of variables in the arguments of the exponential of the Fourier transform that involve $\nabla\theta(x)$, however in this case one leaves behind Fourier transforms and moves into the realm of Fourier Integral Operators [29]. This is a very interesting possibility, but involves complicated inversion formulas and we seek to remain in the context of Fourier-transforms.

Many considerations of the square-root equation in the presence of interactions involving minimal coupling have been noted in the literature [30]. Many articles are critical of the square-root equation because Lorentz invariance is lost in the presence of external fields assuming that minimal coupling is the correct way to introduce interactions. As we have shown above, minimal coupling in the context of the square-root Klein-Gordon operator is inconsistent with local gauge-invariance and the representation of the square-root operator on products of functions using the convolution theorem of Fourier transforms. There exists a representation of interactions in the presence of the square-root Klein-Gordon operator that is both Lorentz-invariant and gauge-invariant. A method of treating interactions that reduces in the limit of local Hamiltonians to minimal coupling was suggested to describe the Aharonov-Bohm effect [31] and developed extensively by S. Mandelstam [32]. This representation of interactions can be traced back to earlier work by

H. Weyl [33] and the introduction of imaginary non-integrable phases [34]. Weyl struggled to distinguish "geometrical" properties from "phase-fields." He obviously had some intuition that the non-Riemannian geometry he was proposing should not strictly be applied to vectors and tensors, but to phases. He was lacking the necessary insight from quantum mechanics at that time to use imaginary phases and apply the results to matter fields. The Mandelstam representation of interactions uses non-integrable phases which have the property that mixed partial derivatives no longer commute.

8. Interacting Fields in the Mandelstam Representation

We now explore a generalization of the theory of interactions applied to the square-root Klein-Gordon theory. The Mandelstam representation of gauge-independent (but path-dependent) fields is given by

$$\psi'(x,t) = \exp\{ie \int_{x_P}^{x} A_\mu \, dx^\mu\} \psi(x,t). \tag{111}$$

Notice that the above equation automatically satisfies gauge-invariance in the form

$$\exp\{ie \int_{x_P}^{x} (A_\mu - \partial_\mu \theta) \, dx^\mu\} e^{ie[\theta(x) - \theta(x_P)]} = \exp\{ie \int_{x_P}^{x} A_\mu \, dx^\mu\}, \tag{112}$$

where $A_\mu - \partial_\mu \theta$ can easily be identified as A'_μ. Here it is obvious that multiplication of ψ by a local phase factor can be incorporated in to the four-vector potential in the form required by local gauge-invariance. The path of integration can be either a space-like or time-like path. In the case of time-like paths we require the exponentiation to be *path-ordered* because the second-quantized theory will involve operators for the four-vector potentials which not commute for time-like separations.

The above product of operators is gauge-invariant by construction. We can use this in the free-field Lagrangian to obtain the interacting case

$$\mathcal{L} = i\psi'^{\dagger}\beta\frac{\partial\psi'}{\partial t} - \psi'^{\dagger}\sqrt{m^2-\nabla^2}\,\psi', \tag{113}$$

with corresponding equations of motion given by

$$\left[i\beta\frac{\partial}{\partial t} - \sqrt{m^2-\nabla^2}\right]\psi' = 0. \tag{114}$$

Sucher [12] has proven the Lorentz-invariance of the free-field square-root equation and has also shown that if one assumes minimal coupling to introduce interactions that Lorentz-invariance is lost. However the above equation of motion is a product of the free-field square-root operator and a Lorentz-covariant path-dependent operator times the free field and the product then would transform under Lorentz transformations $S(\Lambda)$ as

$$S(\Lambda)K_+S^{-1}(\Lambda)S(\Lambda)\exp\{ie\int_{x_P}^{x} A_\mu\, dx^\mu\}S^{-1}(\Lambda)S(\Lambda)\psi(x,t)S^{-1}(\Lambda), \tag{115}$$

where $K_\pm = i\beta\frac{\partial}{\partial t} \mp \sqrt{m^2-\nabla^2}$. Sucher has shown [12] that

$$S(\Lambda)\left[i\frac{\partial}{\partial t} \mp \sqrt{m^2-\nabla^2}\right]S^{-1}(\Lambda) = h\left[i\frac{\partial}{\partial t} \mp \sqrt{m^2-\nabla^2}\right]. \tag{116}$$

The operator h can be computed from commutators of the infinitesimal Lorentz generators and the square-root equation and use of the Campbell-Baker-Hausdorff formula to extend the result to finite Lorentz transformations.

We extend Sucher's proof of Lorentz covariance to the operator $K_{\pm}$ which involves the matrix β. Consider the infinitesimal generators of the Lorentz-transformation $M_{\mu\nu} = x_\mu \frac{\partial}{\partial x^\nu} - x_\nu \frac{\partial}{\partial x^\mu}$. For the case of a infinitesimal boost along the x^i-axis we have to consider commutators N_{10}, where

$$N_{\mu\nu} = [M_{\mu\nu}, K_+]. \tag{117}$$

We make use of Fourier transformations in representing the $\sqrt{m^2 - \nabla^2}$ operator acting on a function. We derive

$$[N_{i0}, i\beta\frac{\partial}{\partial t}] = [-x^i\frac{\partial}{\partial t} - t\frac{\partial}{\partial x^i}, i\beta\frac{\partial}{\partial t}] = i\beta\frac{\partial}{\partial x^i}. \tag{118}$$

Also

$$[N_{i0}, \sqrt{m^2 - \nabla^2}\,] = -\frac{\partial}{\partial t}[x^i, \sqrt{m^2 - \nabla^2}\,]. \tag{119}$$

In order to evaluate the commutator $[x^i, \sqrt{m^2 - \nabla^2}\,]$, we let the commutator act on a function ψ and use integration-by-parts to obtain

$$\begin{aligned}[x^i, \sqrt{m^2 - \nabla^2}\,]\psi =& x^i\sqrt{m^2 - \nabla^2}\,\psi - \\ & \frac{1}{(2\pi)^3}\int e^{ik\cdot(x-y)}\sqrt{m^2 + k^2}[y^i\psi(y)]\,d^3k\,d^3y.\end{aligned} \tag{120}$$

We can write the integral above as

$$\frac{i}{(2\pi)^3}\int \sqrt{m^2 + k^2}\frac{\partial}{\partial k^i}e^{ik\cdot(x-y)}\psi(y)\,d^3k\,d^3y + x^i\sqrt{m^2 - \nabla^2}\,\psi(x). \tag{121}$$

The second term cancels the first term in the commutator $[x^i, \sqrt{m^2 - \nabla^2}\,]$ and by integration by parts we obtain

$$[x^i, \sqrt{m^2 - \nabla^2}\,]\psi(x) = i\frac{\partial}{\partial x^i}[\sqrt{m^2 - \nabla^2}\,]^{-1}\psi(x). \tag{122}$$

Using the definition of K_+ we obtain finally as a generalization of Sucher's transformation for the two-component case

$$\begin{aligned} N_{i0} &= i\beta\frac{\partial}{\partial x^i} - i\frac{\partial}{\partial t}\frac{\partial}{\partial x^i}[\sqrt{m^2 - \nabla^2}\,]^{-1}, \\ &= -i\beta\frac{\partial}{\partial x^i}[\sqrt{m^2 - \nabla^2}\,]^{-1}\,K_+. \end{aligned} \tag{123}$$

The square-root equation, K_+, reappears to the right in Eq. (123) and would also appear to the right in the finite transformation by use of the Campbell-Baker-Hausdorff formula and induction [12]. This proves Lorentz covariance in the free-field case. The interacting case in the Mandelstam representation is a *product* of operators. Notice that each term in the interacting case above transforms in a Lorentz-covariant manner. By inserting the unitary operators that correspond to Lorentz transformations (similarity transformations on the operators) we see that each term in the product transforms by a similarity transformation and the product transforms in a Lorentz-covariant manner. Therefore the Mandelstam approach of introducing interactions does not suffer from loss of Lorentz covariance. Hence we have a reasonable candidate theory that includes interactions and possesses the usual symmetries.

In order to firmly establish the Lorentz invariance of the interacting square-root equation we examine in detail the effects of an infinitesimal Lorentz transformation in the x^i direction (with infinitesimal parameter ϵ)

$$\begin{aligned}
\bar{t} &= t - \epsilon x^i, \\
\overline{x}^i &= x^i - \epsilon t, \\
\frac{\partial}{\partial \bar{t}} &= \frac{\partial}{\partial t} + \epsilon \frac{\partial}{\partial x^i}, \\
\frac{\partial}{\partial \overline{x}^i} &= \frac{\partial}{\partial x^i} + \epsilon \frac{\partial}{\partial t}.
\end{aligned} \tag{124}$$

The above infinitesimal Lorentz transformation can be represented by the operator $U_{it}(\epsilon) = \exp\{-\epsilon M_{it}\}$ where

$$M_{it} = x^i \frac{\partial}{\partial t} + t \frac{\partial}{\partial x^i}. \tag{125}$$

Consider the interacting square-root Klein-Gordon equation

$$\left[i\frac{\partial}{\partial t} - \sqrt{m^2 - \nabla^2} \right] \exp\{ie \int_{x_P}^{x} A_\mu \, dx^\mu\} \psi(x,t) = 0. \tag{126}$$

Clearly the operation of $U_{it}(\epsilon)$ on the product of the Mandelstam line integral and the wavefunction is given by

$$U_{it}(\epsilon) \exp\{ie \int_{x_P}^{x} A_\mu \, dx^\mu\} \psi(x,t) = \exp\{ie \int_{x_P}^{\overline{x}} A_\mu \, dx^\mu\} \psi(\overline{x}, \bar{t}). \tag{127}$$

Consider the transformation on the first operator in Eq. (126)

$$U_{it}(\epsilon) \left[i\frac{\partial}{\partial t} - \sqrt{m^2 - \nabla^2} \right] U_{it}^{-1}(\epsilon). \tag{128}$$

This becomes quite clearly

$$i\frac{\partial}{\partial \bar{t}} - U_{it}(\epsilon)\sqrt{m^2 - \nabla^2}\, U_{it}(-\epsilon), \tag{129}$$

where we have used $U_{it}^{-1}(\epsilon) = U_{it}(-\epsilon)$. Now the infinitesimal Lorentz transformation has the following effect on $\sqrt{m^2 - \nabla^2}$ (we make use of the above commutation relations which hold even in the case of the square-root operator acting on non-integrable functions where the difference of mixed partial derivatives do not vanish)

$$\left[t\frac{\partial}{\partial x^i}, \sqrt{m^2 - \nabla^2}\,\right] = 0,$$

$$\left[x^i\frac{\partial}{\partial t}, \sqrt{m^2 - \nabla^2}\,\right] f(x,t) = \tag{130}$$

$$\frac{\partial}{\partial t}\frac{1}{(2\pi)^3}\int e^{-ik\cdot(x-y)}\frac{(ik_i)}{\sqrt{m^2+k^2}}(f(y,t))\, d^3k\, d^3y.$$

By symmeterizing the time and spatial derivative operations to represent the product of quantum mechanical operators, the effect of an infinitesimal transformation on $\sqrt{m^2 - \nabla^2}$ is

$$U_{it}(\epsilon)\sqrt{m^2 - \nabla^2}\, U_{it}(-\epsilon) = \sqrt{m^2 - \nabla^2} \; - \frac{\epsilon}{2}\left[\frac{\partial}{\partial t}\frac{\partial}{\partial x^i} + \frac{\partial}{\partial x^i}\frac{\partial}{\partial t}\right]\frac{1}{\sqrt{m^2 - \nabla^2}}. \tag{131}$$

This agrees with the first term of a Taylor expansion of $\sqrt{m^2 - \overline{\nabla}^2}$ where

$$\overline{\nabla} = \frac{\partial}{\partial \overline{x}^i}\vec{e}_i + \frac{\partial}{\partial x^j}\vec{e}_j + \frac{\partial}{\partial x^k}\vec{e}_k, \tag{132}$$

and

$$\frac{\partial}{\partial \overline{x}^i} = \frac{\partial}{\partial x^i} + \epsilon\frac{\partial}{\partial t}.$$

Hence the transformed square-root Klein-Gordon equation in the presence of interactions assumes the form in the new coordinate system of

$$\left[i\frac{\partial}{\partial \overline{t}} - \sqrt{m^2 - \overline{\nabla}^2}\right] \exp\{ie\int_{x_P}^{\overline{x}} A_\mu\, dx^\mu\}\psi(\overline{x},\overline{t}) = 0. \tag{133}$$

We clearly see the form-invariance of the equation with respect to infinitesimal Lorentz transformations. The results also hold true for finite Lorentz transformations by application of the Campbell-Baker-Hausdorff formula to exponentiate the infinitesimal result. This clearly demonstrates the Lorentz invariance of the square-root Klein-Gordon equation in the presence of interactions represented by the Mandelstam line integral.

The square-root Klein-Gordon equation is therefore a consistent alternative to the Klein-Gordon equation in the presence of interactions. Both gauge-invariance and Lorentz invariance are preserved in interactions.

The detailed expression involving the kernel for $\sqrt{m^2 - \nabla^2}$ looks like

$$\psi'^{\dagger} \sqrt{m^2 - \nabla^2}\, \psi' = \frac{\psi^{\dagger}(x,t)}{(2\pi)^3} \int e^{ik\cdot(\vec{x}-\vec{y})} \sqrt{m^2+k^2}\, \exp(ie \int_{\vec{x}}^{\vec{y}} A_{\mu}\, dx^{\mu})\, \psi(y,t)\, d^3k\, d^3y, \tag{134}$$

where the line integral $\int_{\vec{x}}^{\vec{y}}$ is taken from x to $-\infty$ along the path containing (x,t) and from $-\infty$ to y along the path containing (y,t) ($\vec{x}$ and $\vec{y}$ are in the hyperplane $t =$ constant.

9. The Aharonov-Bohm effect in the presence of $\sqrt{m^2 - \nabla^2}$

In the case of the Aharonov-Bohm effect one deals with a vector potential of the form $A_{\rho} = 0$, and $A_{\theta} = \frac{e\phi}{2\pi\rho}$, where ϕ is the flux integral (the magnetic field has a finite flux integral but is confined to the z-axis). In this case we can perform the above line integral and obtain a multi-valued function. The initial plane wave at infinity impinges on the flux region and it is easy to verify that the above equation of motion is satisfied for the incoming wave (incident along the x-axis from the right) with the solution $\psi = e^{-ie\phi\theta} e^{-i(\omega_k t + kx)}$, where $\omega_k = \sqrt{m^2+k^2}$ for the relativistic incoming wave. This solution has only positive energy components and therefore we consider solutions of $[i\frac{\partial}{\partial t} - \sqrt{m^2 - \nabla^2}\,]\psi' = 0$. We can look for an eigenfunction expansion for the interacting case and use the property that $\sqrt{m^2 - \nabla^2}\, f_\lambda(x) = \sqrt{\lambda} f_\lambda(x)$ for eigenfunctions of the modified Helmholtz operator. But this is exactly the set of solutions for the general scattering problem in the paper of Aharonov and Bohm

$$\psi = \sum_{m=-\infty}^{\infty} e^{im\theta}[a_m J_{m+e\phi}(k\rho) + b_m J_{-(m+e\phi)}(k\rho)], \tag{135}$$

where ρ is the radial coordinate of the two-dimensional scattering problem and θ is the polar angle. We keep only the terms in the expansion that are regular at the origin. We are then lead by the same arguments as in the original Aharonov-Bohm paper to the result that the scattering amplitude for the asymptotic scattered cylindrical wave in the relativistic case is given [35] by

$$\frac{\sin(\pi e\phi)}{\sqrt{2\pi i k}} \frac{e^{-i\theta/2}}{\cos(\theta/2)}. \tag{136}$$

The cylindrical scattering cross section[#1] is therefore

$$\frac{d^2\sigma}{d\theta dz} = \frac{\sin^2(\pi e\phi)}{2\pi k} \frac{1}{\cos^2(\theta/2)}, \tag{137}$$

where $k = \sqrt{\omega_k^2 - m^2}$.

#1 The cross section in Eq. (22) of [35] needs to be divided by k, the momentum of the incoming particles, in order to have the correct units for a cylindrical cross section.

10. Extensions to Higher Spin

We could imagine that higher spin particles would have Hamiltonians that could be constructed by Pauli's method of modifying p via

$$\vec{p} \rightarrow \vec{\sigma} \cdot \vec{p} = -i\vec{\sigma} \cdot \nabla, \tag{139}$$

where $\vec{\sigma}$ is a spin representation (e.g., for spin-1/2 σ represents the Pauli matrices and could be extended to higher spins by the appropriate representation of $SU(2)$). The square of the operator in Eq. (139) is the product of the 2-by-2 identity matrix times the Laplacian. This is a perfect square

$$\begin{pmatrix} \nabla^2 & 0 \\ 0 & \nabla^2 \end{pmatrix} = (\vec{\sigma} \cdot \nabla)^2. \tag{140}$$

Therefore the operator formula $B = A^2$ implies that B is a perfect square and also implies $A = \sqrt{B}$ as an operator. We have then that

$$\sqrt{-(\vec{\sigma} \cdot \nabla)^2} = \pm i\vec{\sigma} \cdot \nabla. \tag{141}$$

Hence the zero-mass limit of the spin-1/2 square-root operator is a local operator because the argument inside the square-root is a perfect square. This is not the case for the scalar equation. Hence we arrive at the zero-mass limit in the spin-1/2 case

$$i\beta \frac{\partial \psi}{\partial t} = \pm i\vec{\sigma} \cdot \nabla \psi. \tag{142}$$

11. Extensions to Finite Domains

If one restricts the space of functions that the operator $\sqrt{m^2 - \nabla^2}$ acts upon to have specific boundary conditions (i.e., periodic boundary conditions, fixed boundary conditions), then it is possible to define the square-root operator on these functions in terms of integral transforms (i.e., finite Fourier-transforms). If care were taken regarding the even-ness or odd-ness of functions, then finite-sine or finite-cosine transformations could be used as well to descretize $\sqrt{m^2 - \nabla^2}$ for finite domains. Consider the particle in a 1-dimensional box problem. The standing waves have the form

$$\psi_n = A \sin \frac{n\pi x}{L}. \tag{143}$$

It is reasonable to define the action of the square-root operator in this case to be

$$\sqrt{m^2 - \nabla^2}\, \psi_n = \sqrt{m^2 + \left(\frac{n\pi}{L}\right)^2}\, \psi_n. \tag{144}$$

The functions ψ_n form a basis in the space of functions for the 1-dimensional box problem and can be used to extend the definition of $\sqrt{m^2 - \nabla^2}$ to the complete set of functions in this space.

12. Distinction Between the Square-Root and Klein-Gordon Second Quantized Hamiltonians

A serious question comes up regarding the interacting square-root theory and the interacting Klein-Gordon theory: Are these equivalent approaches? The answer is that both theories concern scalar particles and are equivalent in the free-particle case, but *differ in the implementation of interactions to such a degree that they* *are completely distinct theories with different predictions in the presence of interactions.*

We consider a simple example of interactions involving the external Coulomb potential. When one looks in detail at the derivation of the eigenvalue problem of bound-states for the time-independent Klein-Gordon equation in the presence of the Coulomb potential, the time-independent eigenvalue problem for the bound-state is written assuming the square-root representation of the energy operator as follows

$$E\psi = [\sqrt{m^2 - \nabla^2} + V(r)]\psi, \tag{145}$$

where $V(r) = -Ze^2/r$ and r is the radial coordinate for the external Coulomb potential between oppositely charged particles. At this point everything is quite appropriate according to the definition of the operators and the Schrödinger equation. However, the next steps are most important and we shall pay close attention. First the potential, $V(r)$, is placed on the other side of the equation

$$[E - V(r)]\psi = \sqrt{m^2 - \nabla^2}\,\psi, \tag{146}$$

then the eigenfunction ψ is stripped away and the operator equation is "squared"

$$[E - V(r)]^2 = (m^2 - \nabla^2), \tag{147}$$

and finally the "squared" operator is allowed to act on the eigenfunction

$$[E - V(r)]^2\psi = (m^2 - \nabla^2)\psi. \tag{148}$$

This is the form normally used in the textbooks [36] for the Coulomb problem for the time-independent Klein-Gordon equation.

There is a clear lack of consistency in going from Eq. (146) to Eq. (148) since these two equations have *different eigenvalues* and *different eigenfunctions*. In fact Eq. (148) follows from Eq. (146) only if $\sqrt{m^2 - \nabla^2}$ commutes[#2] with $V(r)$, i.e.,

$$\left[\sqrt{m^2 - \nabla^2}\,, V(r)\right] = 0. \tag{149}$$

This can be easily seen by operating from the left on both sides of Eq. (146) with $\sqrt{m^2 - \nabla^2}$. This distinction has been the source of much confusion in the field. Fortunately the distinction between the interacting single-particle Klein-Gordon theory and the square-root Klein-Gordon theory in the presence of the external Coulomb potential [37] have been cleared up in the literature. The most important result of this work is that the eigenvalue spectrum for both the interacting Klein-Gordon equation, Eq. (148), and Eq. (146) agree in the limit of small values of Z, but *disagree* for large values of Z. The external Klein-Gordon equation in the presence of the Coulomb potential becomes *supercritical*[#3] for $Z\alpha = 1/2$ (α is the fine-structure constant), whereas the interacting square-root Klein-Gordon equation becomes supercritical at $Z\alpha = 2/\pi$. This is very interesting because both theories attempt to describe spin-0 particles interacting with the same potential and yet only agree for very weak fields. Hence we conclude that the implementation of interactions has different physical consequences depending on the order which the operators are taken. The effect of ignoring the commutator in Eq. (147) and Eq. (148) leads to Z-dependent disagreements in the spectrum with the discrepancies becoming larger with larger Z.

#2 Gary H. Shoemaker, California State University, Sacramento, private communication.

#3 In QED, any bound state with energy below the Fermi energy $E_{\text{total}} = -m$ is said to be supercritical because it is unstable through spontaneous vacuum decay.

The same thing happens in the case of second quantization. Examination of the transformations in Eq. (39) indicates that there is a close relationship between the Hamiltonian in Eq. (38) and the Klein-Gordon Hamiltonian in either of the forms given in Eq. (40) or the more standard Eq. (41). When no interactions are present one recovers the second quantized Klein-Gordon Hamiltonian. However it is absolutely vital to notice that the transformation (let $\hat{\phi}$ and $\hat{\chi}$ denote the operators for the second-quantized Klein-Gordon Hamiltonian)

$$\begin{aligned} \hat{\phi} &= C^{-1}\phi, \\ \hat{\chi} &= C\chi, \end{aligned} \tag{39}$$

where $C = (m^2 - \nabla^2)^{1/4}$, basically consists of putting in the factor of $\sqrt{\omega_k}$ ($\omega_k = \sqrt{m^2 + k^2}$) into the the denominator of the the square-root Hamiltonian field operators. The $\sqrt{\omega_k}$ factor is essential in the standard Klein-Gordon theory (in the normalization of the second quantized Klein-Gordon field operators) in order to undo the artificial "squaring" of the energy in an effort to represent the Klein-Gordon Hamiltonian as a sum over harmonic oscillators.

Now, the above is only true when <u>no</u> interactions are present. *However, this correspondence does <u>not carry</u> over to the interacting case!* This is a major point of departure between the two theories. This can be easily proven by inserting interactions via the Mandelstam procedure and asking under what conditions do they reduce to the same theory.

The Mandelstam procedure represents interactions via

$$\psi'(x,t) = \mathcal{A}\psi(x,t), \tag{150}$$

where

$$\mathcal{A} = \exp\{ie \int_{x_P}^{x} A_\mu \, dx^\mu\}, \tag{151}$$

and A_μ represents a four-vector potential interacting with the field operator ψ. We ask: What conditions must be satisfied in order that the two interacting theories are equivalent? Let us implement the Mandelstam procedure and examine the interacting Lagrangian

$$\mathcal{L} = \psi^\dagger \mathcal{A}^\dagger i\beta \frac{\partial(\mathcal{A}\psi)}{\partial t} - \psi^\dagger \mathcal{A}^\dagger \sqrt{m^2 - \nabla^2}\, \mathcal{A}\psi, \tag{152}$$

with corresponding equations of motion given by

$$\left[\beta(i\frac{\partial}{\partial t} - eA_0) - \mathcal{A}^\dagger \sqrt{m^2 - \nabla^2}\, \mathcal{A}\right]\psi = 0. \tag{153}$$

This system of equations can be written out in terms of ϕ and χ as

$$\begin{aligned} i\frac{\partial}{\partial t}\phi &= eA_0\phi + \mathcal{A}^\dagger \sqrt{m^2 - \nabla^2}\, \mathcal{A}\chi, \\ i\frac{\partial}{\partial t}\chi &= eA_0\chi + \mathcal{A}^\dagger \sqrt{m^2 - \nabla^2}\, \mathcal{A}\phi. \end{aligned} \tag{154}$$

Clearly we can add or subtract the two systems and obtain

$$i\frac{\partial}{\partial t}\psi^\pm = eA_0\psi^\pm \pm \mathcal{A}^\dagger \sqrt{m^2 - \nabla^2}\, \mathcal{A}\psi, \tag{155}$$

where the + sign holds for the positive energy problem and the − sign holds for negative energy problem. Clearly the positive energy problem is exactly analogous to the original problem in Eq. (145) since in the case of the Coulomb potential with $\vec{A} = 0$ we have $[\sqrt{m^2 - \nabla^2}\,, \mathcal{A}] = 0$.

The square-root Hamiltonian has terms of the form

$$\phi^{\dagger\prime}\sqrt{m^2-\nabla^2}\,\phi' \tag{156}$$

and the Klein-Gordon Hamiltonian has terms of the form

$$\hat{\phi}^{\dagger\prime}\left[m^2-\nabla^2\right]\hat{\phi}'. \tag{157}$$

For this term the transformation in Eq. (39) will not yield equivalence upon integration by parts unless we have the following condition on the commutator

$$\left[(m^2-\nabla^2)^{1/4}, \exp\{ie\int_{x_P}^{x} A_\mu\, dx^\mu\}\right] = 0. \tag{158}$$

Also, the conditions for equivalence between the interacting square-root theory and the Klein-Gordon theory coming from the terms in the Lagrangian with $\hat{\chi}'$ and χ' require in addition to the above commutation rules that

$$\left[(m^2-\nabla^2)^{1/4}, A_0(x,t)\right] = 0. \tag{159}$$

Both of these commutation rules would have to hold for arbitrary fields in order for the second quantized square-root theory to be equivalent to the second quantized Klein-Gordon theory.

Neither of these conditions hold in the general case of arbitrary fields. The only case in which both of these conditions hold is when the four-vector potential is trivial. It is of utmost importance to consider the differences between the square-root Hamiltonian and the second quantized Klein-Gordon theory in the presence of interactions. Also, it should not be surprising to find agreement between these two different approaches for free-fields (no interactions). In fact it is to be expected that the two theories would agree in the non-interacting limit. From the solutions of the single-particle bound state problems we have an indication that the theories are very similar for weak fields, but that the eigenvalue spectra differ the greatest for strong fields. Presumably this would also be manifest for strong field interactions in the second quantized theory as well and indicates where the main differences lie.

Let us summarize the results so far: 1) The single-particle theories for the Klein-Gordon equation and the square-root Klein Gordon equation are both supposed to describe scalar particles but differ in the implementations of interactions which causes disagreements in the eigenspectra of bound states. These theories are only different by the commutator in Eq. (149); 2) The second-quantized theories involve exactly the same operators but also differ by similar commutators. These theories are therefore distinct.

13. Conclusions

We have constructed the commutator of the field operators associated with the classical energy operator $\sqrt{m^2 - \nabla^2}$. This commutator vanishes for space-like separations. The commutator of the quantum field observables associated with local Hermitian operators also enjoys this same property. For the energy density operator, $\psi^\dagger \sqrt{m^2 - \nabla^2}\, \psi$, a weaker condition can be formulated in which only the time-like region contributes to the integral of the commutator over x and x'. Extensions of $\psi^\dagger \sqrt{m^2 - \nabla^2}\, \psi$ were presented in this paper that require commutation relations or anticommutation relations. Therefore, the QFT associated with Hamiltonians constructed from the $\sqrt{m^2 - \nabla^2}$ operator provide a consistent framework to construct a quantized theory of the conventional spin-0 particles with Bose statistics. This is an extension of Pauli's result [1] to the non-local spin-0 case which was excluded from the considerations of his paper on spin and statistics (See [1], page 720. The reason that Pauli did not consider $\sqrt{m^2 - \nabla^2}$ was precisely because this operator acts at finite distances in the coordinate space). We see that regardless of the fact that $\sqrt{m^2 - \nabla^2}$ is non-local, the QFT associated with it and the related Hamiltonian densities $\mathcal{H}_+$ contain operators that satisfy microscopic causality for the associated observable quantities. Hence microscopic causality can be hidden in non-local operators. Also, we present a method of introducing interactions that preserves Lorentz invariance and gauge invariance and indicate why minimal coupling must be abandoned for the square-root equation.

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