

**Second Quantization of the Square-Root
Klein-Gordon Operator, Microscopic
Causality, Propagators, and Interactions.**

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May 13, 1993

Submitted to *Physical Review D*

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). The fact that there is a natural scale in the operator as well as the fact that the single particle theory for the Coulomb potential, $V(r) = Ze^2/r$, yields a different eigenvalue spectrum from either the Dirac Hamiltonian or the Klein-Gordon Hamiltonian indicates that this operator is truly distinct from either of the other two Hamiltonians (all three single-particle Hamiltonians have eigenspectra for the 1s states that converge at small atomic numbers, $Z \rightarrow 0$, but diverge from each other at large Z). We find several possible Hamiltonians associated with $\sqrt{m^2 - \nabla^2}$. Depending on the specific Hamiltonian, it is possible to satisfy the equations of motion with commutators or anticommutators. However, for the scalar case considered, only the Hamiltonian that requires commutation rules has a stable vacuum. We investigate microscopic causality for the commutator of the Hamiltonian density. Also 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. This result extends the application of Pauli's¹ result to the non-local case. Pauli explicitly excluded $\sqrt{m^2 - \nabla^2}$ because this operator acts non-locally in the coordinate space. We investigate the problems with applying minimal coupling to the square-root equation and why this method of interactions should be abandoned in favor of the Mandelstam representation (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 quarks² and again in the general problem of binding in very strong fields.³ The problem of the relativistic string (bosonic strings) also involves the square-root operator⁴ and therefore this problem is especially relevant to modern particle theory in a way that is different than the original context.

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 investigated⁵ 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. Section 8 discusses the Mandelstam representation of interactions and the advantages of the Mandelstam representation over minimal coupling. 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 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

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

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

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

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

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

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

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

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

$$i\frac{\partial\psi}{\partial t} = \sqrt{m^2 - \nabla^2}\psi. \quad (5)$$

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

There are several techniques available to define the square-root Klein-Gordon operator seen on the Right-Hand-Side (RHS) of Eq. (5). We can use path integrals,⁸ semi-groups of operators (functional calculus),⁹ the operator calculus,¹⁰ and also pseudodifferential operators.¹¹

If one considers eigenfunctions of the modified Helmholtz operator

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

then it can be shown in the theory of functional analysis that

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

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

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

(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 referred to as the *symbol* of $p(x, D)$.

Symbols provide a very useful way to work with operators. We can use a multiplicative calculus¹² 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

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

and therefore

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

The operator, $\sqrt{m^2 - \nabla^2}$, is a fractional power of the modified Helmholtz operator $(m^2 - \nabla^2)$. H. Weyl¹³ 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 symbol¹⁴ 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

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

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*.¹⁵ 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 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

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

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,¹⁶ but it has a non-local Lagrangian density. Variation with respect to ψ

results in the complex conjugate equation

$$-i\frac{\partial\psi^*}{\partial t} = \sqrt{m^2 - \nabla^2}\psi^*. \quad (13)$$

The canonically conjugate field variable to ψ is given by

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

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

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

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

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

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

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

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

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

and commutators

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

where the + sign gives the anticommutator and the – sign gives the commutator.

From Eq. (19) we can solve for the products of the fields

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

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

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

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

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

The canonical equations of motion have the form

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

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 property¹⁷

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

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 ψ^\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.

Let us explore the most general plane-wave states associated with the above canonical equations of motion. We expand the field operator into plane-wave states

that contain positive and negative frequencies

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

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

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

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

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

χ and ϕ form a doublet¹⁸ of fields given by

$$\psi = \begin{bmatrix} \phi \\ \chi \end{bmatrix}. \quad (32)$$

The equations of motion are given by

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

where

$$\beta = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}. \quad (34)$$

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

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

and for purely negative frequency states the field has the form

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

The above equations of motion can be derived from the Lagrangian

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

with corresponding Hamiltonian given by

$$\mathcal{H} = \psi^\dagger \sqrt{m^2 - \nabla^2} \psi. \quad (38)$$

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

$$\begin{aligned} \hat{\phi} &= (m^2 - \nabla^2)^{-1/4} \phi, \\ \hat{\chi} &= (m^2 - \nabla^2)^{1/4} \chi. \end{aligned} \quad (39)$$

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

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

which is clearly equivalent to the standard Klein-Gordon Hamiltonian density after

performing the standard integration by parts and ignoring the surface terms at infinity

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

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

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

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

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

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

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

which reduces to

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

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

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

The integral in the above formula¹⁹ can be evaluated to obtain

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

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 its 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 $\epsilon \rightarrow 0$ limit of

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

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

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

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

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

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

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

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

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

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

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

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

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

Let us follow Friedrichs in the evaluation of the Hamiltonian density. We have the

following relations²⁰

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

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

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

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.²¹ 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

Hamiltonian²²

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

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

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

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

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

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

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

We can calculate the commutator

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

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

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

Because

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

we have

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

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

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

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

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

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

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

In the case of the vacuum state, $|\Psi \rangle = |0 \rangle$, 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, $|\Psi \rangle = |k \rangle$, 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

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

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 anti-commutation/commutation laws the above reduces in the special case of operators that satisfy Eq. (73) to

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

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)

$$\begin{aligned} \int \psi^\dagger(x) \overrightarrow{O}_x [\psi(x), \psi^\dagger(x')]_{\pm} \overrightarrow{O}_{x'} \psi(x') d^3 x d^3 x' = \\ \int \psi^\dagger(x) \overrightarrow{O}_x [\psi(x), \psi^\dagger(x')]_{\pm} \overleftarrow{O}_{x'} \psi(x') d^3 x d^3 x'. \end{aligned} \quad (75)$$

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' (spacial 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)

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

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

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

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

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

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 $|\Psi\rangle$ yields

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

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., $|\Psi\rangle = |0\rangle$, 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

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

Also

$$\langle \Psi | : \chi^\dagger \sqrt{m^2 - \nabla^2} \chi : | \Psi \rangle = \int \sqrt{m^2 + k^2} [n_k \mp m_k] d^3k. \quad (82)$$

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

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

The propagator for the above problem satisfies the following equation

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

Let us define the following operator (understood to act in the appropriate dimen-

sional space for the problem at hand)

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

We can multiply both sides of the above equation by

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

to obtain

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

The operator on the 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

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

For negative frequencies we obtain

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

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

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

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

$$\begin{aligned} G_{\pm\omega}^o(x) &= \frac{i}{2}(1 \pm \beta)e^{ipx}, \\ G_{\pm\omega}^i(x) &= \frac{-i}{2}(1 \pm \beta)e^{-ipx}. \end{aligned} \quad (91)$$

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

$$G_+(x - x') = \frac{-i}{2(2\pi)} K_- \left[\begin{array}{l} \sqrt{\frac{m\pi}{2(t^2 - x^2)^{1/2}}} H_{-1/2}^{(1)}(m\sqrt{t^2 - x^2}) \quad |t| > |x| \\ i \sqrt{\frac{2m}{\pi(t^2 - x^2)^{1/2}}} K_{1/2}(m\sqrt{x^2 - t^2}) \quad |x| > |t| \end{array} \right] \quad (92)$$

For negative frequencies we obtain

$$G_-(x-x') = \frac{-i}{2(2\pi)} K_- \left[\begin{array}{l} \sqrt{\frac{m\pi}{2(t^2-x^2)^{1/2}}} H_{-1/2}^{(2)}(m\sqrt{t^2-x^2}) \quad |t| > |x| \\ -i\sqrt{\frac{2m}{\pi(t^2-x^2)^{1/2}}} K_{1/2}(m\sqrt{x^2-t^2}) \quad |x| > |t| \end{array} \right] \quad (93)$$

6.4. STATIONARY 2-DIMENSIONAL PROPAGATOR

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

$$\begin{aligned} G_{\pm\omega}^o(\rho) &= -i(1 \pm \beta)\sqrt{m^2 + p^2} H_0^{(1)}(p\rho), \\ G_{\pm\omega}^i(\rho) &= i(1 \pm \beta)\sqrt{m^2 + p^2} H_0^{(2)}(p\rho). \end{aligned} \quad (94)$$

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

$$G(x) = K_- G_F(x), \quad (95)$$

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

$$\begin{aligned} G_{\pm\omega}^o(r) &= \frac{1}{2(2\pi)^2} (1 \pm \beta) p \frac{e^{ipr}}{r}, \\ G_{\pm\omega}^i(r) &= \frac{1}{2(2\pi)^2} (1 \pm \beta) p \frac{e^{-ipr}}{r}. \end{aligned} \quad (96)$$

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. Breakdown of Minimal Coupling

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

$$\hat{h}(k) = \mathcal{F}[h(x)] = \frac{1}{(2\pi)^{3/2}} \int e^{-ik \cdot x} h(x) d^3x. \quad (97)$$

Then

$$\mathcal{F}[f(x)g(x)] = \frac{1}{(2\pi)^{3/2}} \int \hat{f}(k - \xi) \hat{g}(\xi) d^3\xi. \quad (98)$$

Consider multiplying ψ by a phase that is a function of position.

$$\psi'(x, t) = \exp\{ie\theta(x)\} \psi(x, t). \quad (99)$$

Let $f(x) = \exp\{ie\theta(x)\}$ and consider

$$\sqrt{m^2 - \nabla^2} \psi'(x, t) = \frac{1}{(2\pi)^3} \int e^{ik \cdot x} \sqrt{m^2 + k^2} \int \hat{f}(k - \xi) \hat{\psi}(\xi, t) d^3\xi d^3k. \quad (100)$$

$$\sqrt{m^2 - \nabla^2} \psi'(x, t) = \frac{1}{(2\pi)^3} \int e^{ik \cdot x} \hat{f}(k) \int e^{i\xi \cdot x} \sqrt{m^2 + (k + \xi)^2} \hat{\psi}(\xi, t) d^3 \xi d^3 k. \quad (101)$$

$$\sqrt{m^2 - \nabla^2} \psi'(x, t) = \frac{1}{(2\pi)^{3/2}} \int e^{ik \cdot x} \hat{f}(k) \sqrt{m^2 + (k - i\nabla)^2} \psi(x, t) d^3 k. \quad (102)$$

The square-root operator therefore picks up a convolution over the wave-number in the expansion of the function $f(x)$ (i.e., we operate with a shifted square-root operator on $\psi(x, t)$ and integrate the shifted operator weighted by $\hat{f}(k)$). 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. Therefore in the case of $f(x) = \exp\{ie\theta(x)\}$, we do not expect to see the gradient, $\nabla\theta(x)$, entering the square-root operator. 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. Hence we look to a generalization of the theory of interactions which will be applicable in this case. It is true that one could consider a change of variables in the arguments of the exponentials 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.²³ 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.²⁴ 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, there is no reason to expect minimal coupling to be the correct method of introducing interactions since local

gauge transformations of the field operators are not consistent with pulling the gradients of θ inside the square-root. Rather than abandon the square-root equation as being seriously flawed, we rather abandon minimal coupling and seek a more general representation of interactions that reduces to minimal coupling for local Hamiltonians. Such a representation was used in the Aharonov-Bohm effect²⁵ and developed extensively by S. Mandelstam.²⁶ This representation of interactions can be traced back to earlier work by H. Weyl²⁷ and the introduction of imaginary non-integrable phases.²⁸

8. Interacting Fields in the Mandelstam Representation

The Mandelstam representation of gauge-independent (but path-dependent) fields is given by

$$\psi'(x, t) = \exp\left\{ie \int_{x_P}^x A_\mu dx^\mu\right\} \psi(x, t). \quad (103)$$

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

$$\mathcal{L} = i\psi'^\dagger \beta \frac{\partial \psi'}{\partial t} - \psi'^\dagger \sqrt{m^2 - \nabla^2} \psi', \quad (104)$$

with corresponding equations of motion given by

$$\left[i\beta \frac{\partial}{\partial t} - \sqrt{m^2 - \nabla^2} \right] \psi' = 0. \quad (105)$$

Sucher¹⁰ 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

$$S(\Lambda)K_+S^{-1}(\Lambda)S(\Lambda)\exp\left\{ie\int_{x_P}^x A_\mu dx^\mu\right\}S^{-1}(\Lambda)S(\Lambda)\psi(x,t)S^{-1}(\Lambda), \quad (106)$$

where $K_\pm = i\beta\frac{\partial}{\partial t} \mp \sqrt{m^2 - \nabla^2}$. Sucher has shown¹⁰ that

$$S(\Lambda)\left[i\frac{\partial}{\partial t} \mp \sqrt{m^2 - \nabla^2}\right]S^{-1}(\Lambda) = h\left[i\frac{\partial}{\partial t} \mp \sqrt{m^2 - \nabla^2}\right]. \quad (107)$$

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

$$N_{\mu\nu} = [M_{\mu\nu}, K_+]. \quad (108)$$

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

$$[N_{i0}, i\beta\frac{\partial}{\partial t}] = [-x^i\frac{\partial}{\partial t} - t\frac{\partial}{\partial x^i}, i\beta\frac{\partial}{\partial t}] = i\beta\frac{\partial}{\partial x^i}. \quad (109)$$

Also

$$[N_{i0}, \sqrt{m^2 - \nabla^2}] = -\frac{\partial}{\partial t}[x^i, \sqrt{m^2 - \nabla^2}]. \quad (110)$$

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

$$\begin{aligned} [x^i, \sqrt{m^2 - \nabla^2}]\psi &= x^i \sqrt{m^2 - \nabla^2}\psi - \\ &\quad \frac{1}{(2\pi)^3} \int e^{ik \cdot (x-y)} \sqrt{m^2 + k^2} [y^i \psi(y)] d^3 k d^3 y. \end{aligned} \quad (111)$$

We can write the integral above as

$$\frac{i}{(2\pi)^3} \int \sqrt{m^2 + k^2} \frac{\partial}{\partial k^i} e^{ik \cdot (x-y)} \psi(y) d^3 k d^3 y + x^i \sqrt{m^2 - \nabla^2} \psi(x). \quad (112)$$

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

$$[x^i, \sqrt{m^2 - \nabla^2}]\psi(x) = i \frac{\partial}{\partial x^i} [m^2 - \nabla^2]^{-1} \psi(x). \quad (113)$$

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

$$\begin{aligned} N_{i0} &= i\beta \frac{\partial}{\partial x^i} - i \frac{\partial}{\partial t} \frac{\partial}{\partial x^i} [m^2 - \nabla^2]^{-1}, \\ &= -i\beta \frac{\partial}{\partial x^i} [\sqrt{m^2 - \nabla^2}]^{-1} K_+. \end{aligned} \quad (114)$$

The point is that the square-root equation, K_+ , reappears to the right in Eq. (114) and would also appear to the right in the finite transformation by use of the Campbell-Baker-Hausdorff formula and induction.¹⁰ 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.

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

$$\sqrt{m^2 - \nabla^2}\psi' = \frac{1}{(2\pi)^3} \int e^{ik \cdot (\vec{x} - \vec{y})} \sqrt{m^2 + k^2} \exp\left(ie \int_{\vec{x}}^{\vec{y}} A_\mu dx^\mu\right) \psi(y) d^3k d^3y, \quad (115)$$

where the path of integration in the line integral is in the hyperplane t -constant and along the straight line connecting \vec{x} and \vec{y} .

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

$$\psi = \sum_{m=-\infty}^{\infty} e^{im\theta} [a_m J_{m+e\phi}(k\rho) + b_m J_{-(m+e\phi)}(k\rho)], \quad (116)$$

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 given²⁹ by

$$\frac{\sin(\pi e\phi)}{\sqrt{2\pi i k}} \frac{e^{-i\theta/2}}{\cos(\theta/2)}. \quad (117)$$

The cylindrical scattering cross section^{#1} is therefore

$$\frac{d^2\sigma}{d\theta dz} = \frac{\sin^2(\pi e\phi)}{2\pi k} \frac{1}{\cos^2(\theta/2)}, \quad (118)$$

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

#1 The cross section in Eq. (22) of Ref. 25 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

$$\vec{p} \rightarrow \vec{\sigma} \cdot \vec{p} = -i\vec{\sigma} \cdot \nabla, \quad (119)$$

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. (119) is the product of the 2-by-2 identity matrix times the Laplacian. This is a perfect square

$$\begin{pmatrix} \nabla^2 & 0 \\ 0 & \nabla^2 \end{pmatrix} = (\vec{\sigma} \cdot \nabla)^2. \quad (120)$$

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

$$\sqrt{-(\vec{\sigma} \cdot \nabla)^2} = \pm i\vec{\sigma} \cdot \nabla. \quad (121)$$

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

$$i\beta \frac{\partial \psi}{\partial t} = \pm i\vec{\sigma} \cdot \nabla \psi. \quad (122)$$

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 discretize $\sqrt{m^2 - \nabla^2}$ for finite domains. Consider the particle in a 1-dimensional box problem. The standing waves have the form

$$\psi_n = A \sin \frac{n\pi x}{L}. \quad (123)$$

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

$$\sqrt{m^2 - \nabla^2} \psi_n = \sqrt{m^2 + \left(\frac{n\pi}{L}\right)^2} \psi_n. \quad (124)$$

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. 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's¹ result to the non-local spin-0 case which was excluded from the considerations of his paper on spin and statistics (See Ref. 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.

Acknowledgements

I thank my colleagues Richard Lander and Joe Kiskis at the U.C. Davis Physics Department and also Tepper L. Gill at ComSERC (Howard University, Washington, D.C.) for helpful discussions. This work was supported in part by the Inter-campus Institute for Research at Particle Accelerators (IIRPA) and USDOE grant DE FG03 91ER40674.

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