Single-particle quantum mechanics of the free Klein–Gordon equation with Lorentz violation

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Abstract In spite of its problems with interactions, the first-quantized Klein–Gordon equation is a satisfactory theory of free spinless particles. Moreover, the usual theory may be extended to describe Lorentz-violating behavior, of the same types that exist can in second-quantized scalar field theories. However, because the construction of the theory requires a restriction to positive-energy modes, the Hilbert space inner product and the position operator depend explicitly on the form of the Lorentz violation.

1 Introduction

Einsteinian relativity, encompassing both the special and general theories, elevates symmetries such as local Lorentz invariance to fundamental principles—which underlie both the laws of physics and their mathematical representations. However, almost from the moment when Einstein introduced special relativity in 1905, there have been questions about whether the theory’s Lorentz symmetry is really exact, or whether it might just be an extremely accurate and useful approximation. Since then, the study of apparent symmetries that are ultimately found to be only approximately valid has become a major motif in fundamental physics. Therefore, it is arguably even more natural now than it was in 1905 to consider whether local Lorentz symmetry is also only approximate.

Since the 1990s, thanks to the modernization of effective field theory (EFT), it has become relatively straightforward to lay out a test theory that allows for potential violations of rotation invariance and Lorentz boost invariance, all in a systematic way. The theoretical developments have been followed by a surge in experimental interest in testing Lorentz symmetry, because the EFT approach revealed that there were many more possible forms of Lorentz violation than had previously been appreciated; for decades, large areas of the EFT parameter space had gone effectively unstudied. Thus far, the revived experimental interest has not yielded any convincing positive evidence that Lorentz invariance is not absolute, but precision Lorentz tests remain an important area of fundamental physics research. Part of the reason for this is that the payoff if fundamental Lorentz violation is uncovered is expected to be very high; finding Lorentz symmetry to be broken would be colossally important and would presumably open up whole new vistas for studying the fundamental laws of the universe.

The local effective field theory for describing generalized Lorentz-violating modifications to processes involving standard model fields is now well known [1, 2]. This theory, called the standard model extension (SME), is also capable of describing many forms of CPT violation involving standard model fields that are also stable, unitary, and local, since there are connections between CPT violation and Lorentz violation [3]. The SME can also be expanded to cover gravitation, but the extension to metric gravity introduces many complications that do not appear to exist in the particle sector of the SME, which is a quantum field theory (QFT) much like the standard model—rather than a geometric theory like general relativity (GR), which is thus far only really understood at the classical level. The minimal SME is that subsector of the SME which is expected to be renormalizable, as it contains only the finite number of local, Hermitian, gauge-invariant operators which are constructed from the standard model’s known fermion and boson fields, and which are of mass dimension four or less, making them renormalizable by power counting (so long as they are unitary). The terms in the minimal SME action look very much like those found in the usual standard model action, with the key difference that the new SME operators may exhibit uncontracted Lorentz indices; the coefficients multiplying such operators manifest themselves physically as the components of preferred background vectors and tensors. In many situations, the minimal SME is the most natural test theory in which to analyze the results of experimental tests of Lorentz invariance and CPT.

The SME is a field theory, but a great deal may be learned about the physics of the minimal SME by looking at simpler physical theories with the same characteristic Lorentz-violating kinematics. The goal of this paper is to extend this kind of study into a new area—by looking at Lorentz violation in a first-quantized Klein–Gordon theory. This is a timely undertaking, since there have

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In fact, the full classical single-particle Lagrangian fermionic dispersion relation in the minimal SME, corresponding to the EFT Lagrange density \( L \) of products in \( \Lambda_{ae} \) backgrounds [4–11]. The Klein–Gordon equation has well-known problems that make it unsuitable as a relativistic generalization of the single-particle Schrödinger equation—at least in the presence of interactions. However, the noninteracting first-quantized Klein–Gordon theory is completely well behaved, although it has a number of potentially counterintuitive features.

This paper is organized as follows. In Sect. 2, we examine, by way of comparison, the use of single-particle classical Lagrangians with Finsler structures in velocity space as descriptions of Lorentz violation. These have proven to be useful mathematical models, but they are, at present, fundamentally incomplete—capable of providing a full description only of free (or nearly free) particle dynamics. With this in mind, we move in Sect. 3 to another theory that is potentially useful, yet incomplete, because it is also incapable of handling interactions. This is the single-particle Klein–Gordon theory that is the main focus of the paper. In Sect. 4, we look particularly at the structure of the position operator in the Lorentz-violating Klein–Gordon theory. The operator has an unusual structure even in the absence of Lorentz violation, and the broken Lorentz symmetry adds further complications. Finally, Sect. 5 summarizes our conclusions and avenues for further research.

2 The case of Finsler geometry

The rise in interest in Finsler geometry as a formalism for describing Lorentz violation provides some key context for the later main focus of this paper. One important observation about Lorentz-violating theories was that explicit Lorentz violation is not generally compatible with the general theory of relativity—or, more generally, with any theory in which gravitational and cosmographic effects are manifestations of spacetime being a curved pseudo-Riemannian manifold [12]. There is not, in general, room to augment such geometrical theories with a form local Lorentz violation that affects particle movement, because one of the essential feature of geometrodynamics is that test particles’ spacetime trajectories are the geodesics of the manifold. Unless stringent further conditions are met, the Lorentz violation is inconsistent with Riemann (or Riemann-Cartan) geometry. Those stringent conditions can be satisfied if the Lorentz symmetry breaking arises spontaneously, or when the texture of the Lorentz violation takes other special forms [13–16]. However, to study explicitly broken Lorentz symmetry in a nontrivial spacetime background typically requires generalization to manifolds that have more structure than just a Riemannian metric and Cartan spin connection.

The most obvious generalizations of this sort are to Finsler manifolds. The qualitative connection between local Lorentz breaking and Finsler structure has been recognized for quite a long time—since well before the development of the SME. However, with the publication of the “no-go” result [12] for explicit violation in Riemann-Cartan spacetimes, there was naturally a growth of interest in exploring this connection more fully. Unfortunately, Finsler manifolds are very challenging objects to study, and the mathematical tools that are used for studying QFT in Minkowski or Riemannian spacetimes are not generally available in the Finsler case. Most of the fundamental fields in the standard model are spinor fields or gauge fields, which are defined on particular bundles—more complicated than the tangent bundle—in curved spacetimes. Satisfactory analogues of the spinor and gauge bundles on Finsler manifolds may or may not exist, and this means that it is very difficult to make useful statements about the behavior of quantized fields in Finsler geometries.

Even so, there has been quite a bit of interesting work done on the physics of motion in Finsler spacetimes with nontrivial Lorentz-violating structures in momentum space. This research has primarily focused on the motion of classical particles with Lorentz-violating free dynamics. For example, it is possible to use a Finsler structure to describe the motion of a particle with a nonstandard energy-momentum relation involving two preferred background four-vectors \( a \) and \( e \) [17],

\[
(p^{\mu} - d^{\mu})(p_{\mu} - a_{\mu}) - (m - e^{\mu} p_{\mu})^2 = 0; \tag{1}
\]

the same dynamics are produced by a classical one-particle Lagrangian with the Finsler-like structure [18]

\[
L_{ae} = -\frac{m - e \cdot a}{\sqrt{1 - e^2}} \sqrt{\dot{x}^2 + \frac{(e \cdot \dot{x})^2}{1 - e^2} + \left(-a + m - e \cdot a\right) \cdot \dot{x}. \tag{2}
\]

Here \( \dot{x} \) is an appropriately defined four-velocity. The dispersion relation (1) is a special case of the most general spin-independent fermionic dispersion relation in the minimal SME, corresponding to the EFT Lagrange density

\[
L_{ac} = \tilde{\psi} \left[i (\partial_{\mu}) (\gamma_{\mu} + \gamma^{\mu} \gamma_5 + e^{\mu} + i f^{\mu \nu} \gamma_5) - (m + a^{\mu} \gamma_5) \right] \psi. \tag{3}
\]

In fact, the full classical single-particle Lagrangian \( L_{ac} \) that produces the same dispersion relation as for the on-shell field excitations of \( L_{ac} \) is known, but it is an extremely complicated generalization of (2). For the theory with just a \( c \) tensor background, the dispersion relation is instead

\[
(\eta^{\mu \nu} + 2 c^{\mu \nu} + e^{\mu \nu} c_{\alpha}^{\nu} p_{\rho} - m^2) = (p^{\mu} + c^{\mu \nu} p_{\nu}) (p_{\mu} + c_{\rho}^{\mu} p_{\rho}) - m^2 = 0. \tag{4}
\]

Incorporating a \( c \) term into the single-particle \( L \) simply entails, at leading order, replacing the \( \eta^{\mu \nu} \) implicit in the four-vector dot products in \( L_{ae} \) with \( \eta^{\mu \nu} + \frac{1}{2} c^{(\mu \nu)} \), where \( c^{(\mu \nu)} = e^{\mu \nu} + e^{\nu \mu} \) is the symmetrized form of the background.
Even more impressively, this approach can also be used to describe the motion of particles with internal degrees of freedom like spin. The classical particle Lagrangians [18, 19],
\[ L_b = -m\sqrt{\dot{x}^2} \pm \sqrt{(b \cdot \dot{x})^2 - b^2 \dot{x}^2} \] (5)
dictate the dynamics of a free particle whose dispersion relation has two branches,
\[ (p^2 - b^2 - m^2)^2 - 4(b \cdot p)^2 + 4b^2 p^2 = 0, \] (6)
corresponding to the energy-momentum relations for a SME fermion field with a $b$ term
\[ \mathcal{L}_b = \bar{\psi} (i\gamma^\mu \delta_{\mu} - m - b^\mu \gamma_\mu) \psi \] (7)
in the free-field action. This provides an adequate description of the center of mass motion of a spinning particle. More elaborate constructions may be used to create classical Lagrangians for point particles with other types of Lorentz violation [20–22], including going beyond the minimal SME to consider higher-dimensional field operators [23, 24]. It is possible to draw interesting conclusions about the global structures of these Finsler spaces, with the modified dispersion relations living on their tangent bundles, and there have been some first steps toward understanding vector bundles [25–27]. What is missing, however, is a dynamical picture of how a particle may pass from one branch of the dispersion relation to another—in other words, the dynamics of a spin transition. For all the successes of the theories’ modified dispersion relations, this is a very serious deficiency. The lack of full knowledge of how to place spin field bundles on the Finsler spacetime means that there is, as yet, no way to study their relativistic dynamics in the SME-Finsler framework.

3 Klein–Gordon theory of a free particle

As previously noted, most of the fundamental fields in the standard model are spinor or gauge fields. However, the standard model does have a scalar sector, in the form of the Higgs. While fields with spin “live” in nontrivial bundles on curved spacetimes, the scalar sector is simpler. In particular, there are fewer possible forms of minimal SME Lorentz violation, since a scalar field has no intrinsic spin direction. In fact, the free dynamics of a simple complex scalar species are equivalent to those of a fermion field described by $\mathcal{L}_\text{ferm}$ with only the $a$ and $c$ tensors nonzero; and for a real scalar field, only a nonzero $c$ is possible. The dispersion relation for such a scalar field in Riemann-flat spacetime takes the fairly simple form (which can also be derived from a particularly simple Finsler structure [19])
\[ (\eta^{\mu\nu} + k^{\mu\nu}) p_\mu p_\nu - \mu^2 = 0. \] (8)
This is the energy-momentum relation for the scalar QFT with Lagrange density
\[ \mathcal{L} = \frac{1}{2} (\partial^\mu \phi)(\partial_\mu \phi) + \frac{1}{2} k^{\mu\nu} (\partial_\mu \phi)(\partial_\nu \phi) - \frac{1}{2} \mu^2 \phi^2. \] (9)
It is evident that, at leading order, $k^{\mu\nu}$ is the fermionic equivalent of $c^{(\mu\nu)}$; moreover, the exact equivalence between boson $k$ and fermion $c$ persists, albeit with slight adjustments, to all orders. (The best way to demonstrate this is through the use of a supersymmetry equivalence between Lorentz-violating scalar and spinor fields [28].) The slight differences between the dispersion relations with $k^{\mu\nu}$ and $c^{(\mu\nu)}$ arise from the fact that while $c$ may be assumed to be symmetric only at leading order, it is manifest from (9) that the antisymmetric part of $c$ does not actually contribute to the action at any order.

In order to second quantize the theory defined by (9), it is often useful to rescale the field $\phi$ and the mass parameter $\mu$ so that the Lagrange density contains no nonstandard second time derivatives. This may be done because a term proportional to $\eta^{\mu\nu}$ may be subtracted from $k^{\mu\nu}$ and transferred to the conventional Klein–Gordon kinetic term in (9). After rescaling $\phi$ and $\mu$, the Lagrangian still has the general form (9), albeit with different specific values for the components of the background tensor $k$. To eliminate any nonstandard $\partial^\mu \phi$ derivatives specifically, the subtraction yields an effective $k^{\mu\nu}$ of the form $k^{\mu\nu} - k^{00} \eta^{\mu\nu}$. Although our concern here will not be with the second-quantized field theory, it will typically be convenient to restrict attention to modified Klein–Gordon theories in which $k^{00} = 0$. Moreover, if there is only a single field in the theory [as in (9)], it is actually possible, via an affine redefinition of the coordinates, to eliminate all the $k^{\mu\nu}$ coefficients from the action. This would render the Lorentz violation trivial (and, in any case, would only work in an interacting theory for a single field sector), so we shall not follow that procedure. Without transforming the coordinates in this way, it is not, in general, possible to find a Lagrangian equivalent to (9) in which $k^{00} = 0$. (This contrasts with an analogous fermionic theory with $c^{00}$ coefficients, which can be eliminated via a linear transformation in spinor space—or equivalently, a change in the representation of the Dirac matrices. The difference is that no such adjustable matrix structure exists in the Klein–Gordon theory.) However, we shall often impose the additional $k^{00} = 0$ restriction, in order to produce tractable and straightforwardly interpretable expressions, since separating out the positive- and negative-energy state manifolds in a theory with time and space derivatives mixed by $k^{j0} \neq 0$ may introduce additional nontrivial complications.

Many previous studies of the dynamics of single particles with nontrivial Finsler structures in their momentum space have treated theories that are essentially interaction free, except for the local Lorentz violation effects associated with their Finsler metrics.
However, if attention is to be restricted to free theories, there is another kind of free theory, which (although it is little discussed today) lies in an intermediate position between classical theories of point particles and second-quantized field theories. This is the first-quantized scalar theory with a relativistic wave function that satisfies the Klein–Gordon equation. Of course, the first-quantized Klein–Gordon theory has insurmountable problems in the presence of interactions, but the free theory is perfectly well behaved, although it has some potentially counterintuitive features. The Lorentz-violating version of the first-quantized free Klein–Gordon theory will be the subject of the remainder of this paper. Since a scalar field "lives" on the spacetime manifold itself, understanding its dynamics only requires knowledge of the structure of the tangent bundle, which is well defined in Finsler theories. As noted, a Lagrange density like (9) has itself a straightforward relationship to a Finsler structure. The first-quantized version of the theory consequently offers a different window onto a theory with a Finsler-like structure distorting the momentum space—a viewpoint which should be complementary to those previous analyses that have looked at the motion of single classical point masses.

For a single-particle wave function satisfying the usual relativistic Klein–Gordon equation,

\[ (\partial_\mu \partial^\mu + \mu^2)\psi = 0, \] (10)

there is a conserved vectorial current

\[ j^\mu = \frac{i}{2\mu} \left[ \psi^* (\partial^\mu \psi) - (\partial^\mu \psi^*) \psi \right]. \] (11)

At nonrelativistic energies \( E \approx \mu \), the time component reduces to \( j^0 \approx \psi^* \psi \). However, for wave functions that contain negative-energy Fourier components, the purported probability density \( j^0 \) need not be positive, meaning that Born's standard probability interpretation of the wave function \( \psi \) fails completely. In fact, because the Klein–Gordon equation is second order in time, it is possible to specify a Cauchy initial value problem with \( \psi \) chosen arbitrarily (subject to appropriate differentiability conditions, of course); consequently, \( j^0 \) may actually be made arbitrarily negative in the vicinity of any given point.

The historical solution to this problem was, of course, to replace the second-order Klein–Gordon equation with the first-order Dirac equation—thus eliminating the potentially negative time derivative terms in \( j^0 \). However, while some of the glaring failures of the probability current interpretation in Klein–Gordon quantum mechanics are avoided, the single-particle Dirac theory of course has problems of its own with the probability current (problems which typically appear in the presence of very strong interactions).

Yet there is sometimes another way of addressing the problem of the negative probabilities that crop up in the first-quantized Klein–Gordon theory. The alternative approach only works as a theory of a noninteracting Klein–Gordon particle, but we understand that even noninteracting Lorentz-violating theories may be quite instructive; such was the case with the free particle theories based on Finsler structure Lagrangians. The alternative solution is simply to consider wave functions with entirely positive-frequency Fourier components, the purported probability density \( j^0 \) need not be positive, meaning that Born’s standard probability interpretation of the wave function \( \psi \) fails completely. In fact, because the Klein–Gordon equation is second order in time, it is possible to specify a Cauchy initial value problem with \( \psi \) chosen arbitrarily (subject to appropriate differentiability conditions, of course); consequently, \( j^0 \) may actually be made arbitrarily negative in the vicinity of any given point.

The modified Klein–Gordon equation with the dispersion relation (8) is

\[ \left[ (\eta^{\mu\nu} + k^{\mu\nu}) \partial_\mu \partial_\nu + \mu^2 \right] \psi = 0. \] (12)

There is a modified current conservation equation in this theory, with the current

\[ j^\mu = -\frac{1}{2\mu} \left\{ \psi^* \left( \partial^\mu \psi + k^{\mu\nu} \partial_\nu \psi \right) \right\} \] (13)

generalizing (11). Taking the divergence of this quantity,

\[ \partial_\mu j^\mu = -\frac{1}{2\mu} \left\{ \partial_\mu \left( \psi^* \left( \eta^{\mu\nu} + k^{\mu\nu} \right) \partial_\nu \psi \right) \right\} \] (14)

and applying the modified Klein–Gordon Eq. (12), it is clear that the expression in French brackets must be real, and hence \( \partial_\mu j^\mu = 0 \).

If there is to be a first-quantized theory, the probability density must be the time component of the current, \( \rho \propto j^0 \), so that \( \int d^3x \rho(x) \) is a conserved quantity which may be normalized to unity. This, in turn, sets the (unnormalized) inner product between two wave functions \( \psi_1 \) and \( \psi_2 \).

\[ \langle \psi_2 | \psi_1 \rangle = i \int d^3x \left\{ \psi_2^* \left[ (\eta^{00} + k^{00}) \partial_0 \psi_1 \right] - \left[ (\eta^{00} + k^{00}) \partial_0 \psi_2^* \right] \psi_1 \right\}. \] (15)

(This expression is for a fixed time \( x_0 \), but in general, the integration may be pushed to an arbitrary spacelike hypersurface \( \Sigma \).)

Provided \( k \) is sufficiently small, there should not be problems with negativity in this theory. Moreover (and more precisely), in the theory in which only the space-space components \( k^{ij} \) of the background are nonvanishing, the expression for \( \langle \psi_2 | \psi_1 \rangle \) is the same as in the standard Lorentz-invariant theory.
Continuing henceforth in the restricted \( k^{\mu 0} = 0 \) theory, it is clear that the plane waves of positive energy, which satisfy \( i \delta \left\{ \psi^* \psi \right\}_ ++ = 0 \), obey the equation

\[
i \partial^0 \psi = \sqrt{\mu^2 - \nabla^2 + k^j \nabla_j \nabla_l} \psi.
\]

The square root operator should be understood in Fourier (three-momentum) space, such that if

\[
\psi(x) = \int d^3 \rho \ e^{i \vec{p} \cdot \vec{x}} \chi(\vec{p}, x_0),
\]

then \( \chi(\vec{p}, x_0) \) obeys

\[
i \partial^0 \chi(\vec{p}, x_0) = \omega(\vec{p}) \chi(\vec{p}, x_0) = \sqrt{\mu^2 + \vec{p}^2 - k^j p_j} \chi(\vec{p}, x_0).
\]

Although Eq. (16) is nonlocal in space, it is first order in time. This alleviates the problem with positivity of \( j^0 \), because it is no longer possible to set \( \psi \) as an independent initial condition.

To form a wave packet out of these positive-energy plane waves, we may take a four-dimensional Fourier expansion,

\[
\psi(x) = \frac{\sqrt{2}}{(2\pi)^{3/2}} \int \frac{d^4 p}{\sqrt{2} p_0} e^{-ip \cdot x} \delta \left( p^2 + k^j p_j - \mu^2 \right) \theta(p_0) \Psi(p).
\]

The \( \delta \)-function and \( \theta \)-function ensure that the plane wave components each obey the Lorentz-violating Klein–Gordon equation and have positive energy; the multiplicative constants are chosen for convenience. To obtain a more convenient expression in terms of the Fourier-space \( \Psi(p) \), we may carry out the \( p_0 \) integration via

\[
\delta \left( p_0^2 - \omega(\vec{p}) \right) \theta(p_0) = \frac{1}{2\omega(\vec{p})} \left[ \delta(p_0 - \omega(\vec{p})) + \delta(p_0 + \omega(\vec{p})) \right] \theta(p_0) = \frac{1}{2\omega(\vec{p})} \delta(p_0 - \omega(\vec{p})),
\]

so that

\[
\psi(x) = \frac{1}{(2\pi)^{3/2}} \int \frac{d^3 p}{\sqrt{2} p_0} e^{-ip \cdot x} \Psi(p),
\]

where \( p_0 = +\omega(\vec{p}) \) is now considered a function of the three-momentum \( \vec{p} \). As a result, the Fourier coefficients \( \Psi(p) \) may also be written as a function \( \Psi(\vec{p}) \) of the three-momentum only, as there is exactly one \( p_0 > 0 \) value that corresponds to any given \( \vec{p} \).

Returning to the inner product (15)—still in the \( k^{\mu 0} = 0 \) case—it is now possible to simplify

\[
\langle \psi_2 | \psi_1 \rangle = \int d^3 x \left\{ \Psi^*_2(x) \left[ \sqrt{\mu^2 - \nabla^2 + k^j \nabla_j \nabla_l} \Psi_1(x) \right] + \left[ \sqrt{\mu^2 - \nabla^2 + k^j \nabla_j \nabla_l} \Psi^*_2(x) \right] \Psi_1(x) \right\}
\]

by inserting the Fourier transforms (21), to yield

\[
\langle \psi_2 | \psi_1 \rangle = \frac{1}{2(2\pi)^3} \int \frac{d^3 x \ d^3 p_2 \ d^3 p_1}{p_0(p_2)p_0(p_1)} \left\{ e^{i p_2 \cdot x} \Psi^*_2(\vec{p}_2) \left[ \sqrt{\mu^2 - \nabla^2 + k^j \nabla_j \nabla_l} e^{-i p_1 \cdot x} \Psi_1(\vec{p}_1) \right] + \left[ \sqrt{\mu^2 - \nabla^2 + k^j \nabla_j \nabla_l} e^{i p_2 \cdot x} \Psi^*_2(\vec{p}_2) \right] e^{-i p_1 \cdot x} \Psi_1(\vec{p}_1) \right\}.
\]

Collecting common terms and picking out the \( \delta \)-function \( (2\pi)^{-3} \int d^3 x \ e^{i(p_2 - p_1) \cdot x} \), we finally reach

\[
\langle \psi_2 | \psi_1 \rangle = \int \frac{d^3 p}{p_0} \Psi_2^*(\vec{p}) \Psi_1(\vec{p}).
\]

In this form, no Lorentz-violation coefficient \( k \) appears; however, the Lorentz violation is still present in a fundamental way. The Lorentz-violating dispersion relation \( p_0 = +\omega(\vec{p}) \) enters as a weight in the integration. So the inner product—as, for example, expanded in plane waves (24)—depends on the character of the Lorentz violation!

Plane waves with position-independent amplitudes are, of course, not strictly normalizable. However, we may adopt a standard \( \delta \)-function normalization for these eigenstates of the rigged Hilbert space. With a continuum normalization

\[
\langle \psi_{\vec{p}} | \psi_{\vec{p}} \rangle = p_0 \delta^3(\vec{p}_1 - \vec{p}_2),
\]

the plane waves should be

\[
\psi_{\vec{p}} = \frac{e^{-ip \cdot x}}{\sqrt{2(2\pi)^3}}
\]
up to an overall phase. However, this means that the closure relation

$$\sum_p |\psi_{\vec{p}}(x_1)\rangle \langle \psi_{\vec{p}}(x_2)| = \frac{1}{2(2\pi)^3} \int \frac{d^3p}{p_0} e^{-ip \cdot (x_1 - x_2)}$$

(27)
is not a $\delta$-function—even when the times are equal, $x^0_1 = x^0_2$. The momentum sum on the left-hand side of the expression (27) is, of course, actually implemented as an integral, but the expression on the right-hand side is straightforward; its form is dictated by requiring that when sandwiched between an additional bra on the left and ket on the right, the resulting inner products take the form (24).

Note, however, that the principal peculiarity of (27)—that the closure relation does not yield a $\delta$-function—is not a consequence of the Lorentz violation, but of the fact that the positive-energy modes of the Klein–Gordon operator do not span the full space of square-integrable spacetime functions. There is the same discrepancy in the Lorentz-symmetric theory. However, the positive-energy modes do span a Hilbert space $\mathcal{H}_+$ of free particle modes, in which the plane waves are manifestly eigenstates of the three-momentum operator.

4 The position operator

Where the operator algebra is really modified is with the introduction of the position operator. One of the strangest properties of having a theory with these atypical position operators is that spatially localized wave functions are not described by $\delta$-functions [a parallel to the lack of a $\delta$-function in (27)]. Instead, a different, more general characterization of spatially localized states is required.

Because the inner product in the momentum representation (27) contains the nontrivial weighting factor $1/p_0$, the operator $i\vec{\nabla}_{\vec{p}}$ is not self-adjoint and so cannot be the representation of the physical position observable $\vec{x}$.

$$\langle \psi_2 | x_j | \psi_1 \rangle = i \int \frac{d^3p}{p_0} \Psi_2^*(\vec{p}) \frac{\partial}{\partial p_j} \Psi_1(\vec{p})$$

(28)

$$= \int \frac{d^3p}{p_0} \left[ -i \frac{\partial}{\partial p_j} + i \frac{p_j - k_j p^l}{\mu^2 + \vec{p}^2 - k^m p_m} \right] \Psi_2^*(\vec{p}) \Psi_1(\vec{p})$$

(29)

$$\neq \langle x_j | \psi_2 | \psi_1 \rangle.$$  

(30)

Instead, the self-adjoint part of $\vec{x}$ should be defined to be the position operator (recall that we are still working in the restricted theory in which $k^{\mu 0} = 0$),

$$x^op_j = i \frac{\partial}{\partial p_j} - i \frac{p_j - k_j p^l}{2 \mu^2 + \vec{p}^2 - k^m p_m}.$$  

(31)

The form of the position operator depends explicitly on the Lorentz-violating background!

This is obviously a generalization of the result from the Lorentz-invariant ($k^{\mu v} = 0$) first-quantized Klein–Gordon theory,

$$\vec{x}^op = i \vec{\nabla}_{\vec{p}} - \frac{i}{2} \frac{\vec{p}}{\mu^2 + \vec{p}^2}.$$  

(32)

The understanding that this was the proper quantum-mechanical position operator for the single-particle Klein–Gordon theory originally arose out a broader study of “center-of-mass” operators in relativistic quantum mechanics [30–32]. Interest in this problem was, unsurprisingly, more focused on the more complicated and physically important first-quantized Dirac theory. In that case, careful analyses led to the identification of the Zitterbewegung—free “position operator—which is usually derived using a Foldy–Wouthuysen transformation [33, 34]—by different means. (The role of Zitterbewegung and how to separate it from the mean velocity in the Lorentz-violating Dirac theory have previously been discussed in Ref. [35].)

In the single-particle Dirac theory, the Zitterbewegung (and the procedure for eliminating it to extract the mean position operator) are also inseparable from the theory’s energy-momentum relation. The high-frequency oscillations that are part of the dynamics (and other related quirks, such as the components of the formal velocity operator having only $\pm 1$ eigenvalues, and the velocity components not commuting with one-another) appear because of interference between positive- and negative-frequency components in a well-localized wave function. To free the physical operator from the Zitterbewegung we will thus necessarily require deriving a new mean operator that depends on the dispersion relation—similar to the way that $\vec{x}^op$ invokes $o(\vec{p})$ and its gradient, whereas the naive operator $i\vec{\nabla}_{\vec{p}}$ does not.

In the Klein–Gordon theory, the position operator may be characterized axiomatically [29] (although there are much more recent criticisms of that approach [36]—related, in part, to the lack of connection to a satisfactory interacting theory), and one of the conditions that characterizes the spatially nonlocal position operator (32) is that physical states localized at different spatial points must be orthogonal, in spite of the fact that such localized wave functions are not $\delta$-functions with point-like support. We shall now look at the Lorentz-violating generalization of this spatial orthogonality characterization.
A necessary condition for the theory to be interpretable is that two states localized at different positions at a common time \( x_0 = 0 \) be orthogonal. Assuming that appropriately localized states do exist, the states centered on different points must be spatial translates of one-another. Starting with a state \( |\psi_{x_1}\rangle \) with momentum-space representation \( (\Psi) \) the \( p \)-space representation of a translation by \( \vec{x}_2 - \vec{x}_1 \) is simply \( e^{-i\vec{p}(\vec{x}_2 - \vec{x}_1)} \), so \( \Psi_{\vec{x}_2}(\vec{p}) = e^{-i\vec{p}(\vec{x}_2 - \vec{x}_1)}\Psi_{\vec{x}_1}(\vec{p}) \), and the overlap of the two states is

\[
\delta^3(\vec{x}_2 - \vec{x}_1) = \langle \psi_{\vec{x}_2} | \psi_{\vec{x}_1} \rangle = \int \frac{d^3p}{p_0} e^{i\vec{p}(\vec{x}_2 - \vec{x}_1)}\Psi_{\vec{x}_2}(\vec{p})\Psi_{\vec{x}_1}(\vec{p}).
\]

(33)

This is indeed a \( \delta \)-function if \( |\Psi_{\vec{x}_1}(\vec{p})|^2 = (2\pi)^{-3}p_0 \).

This fixes the magnitude of the momentum-space wave function of a spatially localized state. To get the phase, we must apply the eigenvalue condition for \( \vec{x}_\text{op} \) directly. [In the Lorentz-invariant theory, it is possible to obtain the full \( |\Psi_{\vec{x}_1}(\vec{p})|^2 \) in a different way, by imposing physical \( O(3) \) invariance around \( \vec{x}_1 \). However, that obviously does not apply to the theory with the Lorentz-violating \( k \) term.] Setting \( \Psi_{\vec{x}_1}(\vec{p}) = (2\pi)^{-3/2}p_0(\vec{p}) e^{i\alpha(\vec{x}, \vec{p})} \), the eigenvalue equation

\[
\left( i\frac{\partial}{\partial p}\right) - \frac{i}{2}\frac{p_j - k_{jl}p_l}{p_0(\vec{p})} \sqrt{p_0(\vec{p})} e^{i\alpha(\vec{x}, \vec{p})} = x_j \sqrt{p_0(\vec{p})} e^{i\alpha(\vec{x}, \vec{p})},
\]

implying simply that \( \alpha(\vec{x}, \vec{p}) = -i\vec{p} \cdot \vec{x} \) (plus an irrelevant constant), since the second term in \( \vec{x}_\text{op} \) arose as precisely \(-\frac{1}{2}\) times what was needed to cancel \( i\frac{\partial}{\partial p_j} \) acting on \( 1/p_0 \). So the Fourier representation of the localized spatial state is

\[
\Psi_{\vec{x}_1}(\vec{p}) = (2\pi)^{-3/2} \left( \frac{\mu^2 + \vec{p}^2 - k_{jl}p_j p_l}{p_0(\vec{p})} \right)^{1/4} e^{-i\vec{p}\cdot\vec{x}},
\]

(35)

and the amplitude for finding a particle in the state \( |\psi\rangle \) at a particular position \( \vec{x} \) is

\[
\langle \psi_{\vec{x}} | \psi \rangle = \frac{1}{(2\pi)^{3/2}} \int d^3p \frac{e^{-i\vec{p}\cdot\vec{x}}}{\left(\mu^2 + \vec{p}^2 - k_{jl}p_j p_l\right)^{1/4}} \Psi(\vec{p}).
\]

(36)

The wave function in configuration space is, as previously noted, not a \( \delta \)-function. It does not need to be completely localized, since the probability density is not \( |\psi(x)|^2 \). Instead, for a wave function localized at the origin (still on the time slice \( x_0 = 0 \)), the formula is

\[
\psi_0(x_0 = 0, \vec{x}) = \frac{1}{\sqrt{2(2\pi)^3/2}} \int d^3p \frac{e^{i\vec{p}\cdot\vec{x}}}{\sqrt{p_0 e^{i\vec{p}\cdot\vec{x}}}.
\]

(37)

A very similar integral to this one (differing only by the power of \( p_0 \) in the integrand) was previously evaluated in Ref. [37], in the context of finding the Yukawa potential mediated by a scalar field with \( k \)-type Lorentz violation. The integrals may be related to their Lorentz-invariant \( (k = 0) \) versions using a linear change of coordinates. (This is actually closely related to the change of coordinates, discussed in Sect. 3 that could be used to remove \( k \) from the field theory Lagrangian.) Define a matrix \( K \) with \( K_{jl} = \delta_{jl} - k_{jl}; \) \( K \) is symmetric and, presuming the Lorentz violation is small, also positive definite. By making an orthogonal rotation of the integration variables \( \vec{p} \), we may diagonalize it, and in the rotated coordinates, the Fourier transform becomes

\[
\psi_0(0, \vec{x}) = \frac{1}{\sqrt{2(2\pi)^3/2}} \int d^3p \frac{e^{i\vec{p}\cdot\vec{x}}}{\left(\mu^2 + K_{11}p_1^2 + K_{22}p_2^2 + K_{33}p_3^2\right)^{1/4}}.
\]

(38)

Another linear transformation will suffice to bring the integral into a known form, rescaling \( \vec{p}_j = \sqrt{K_{jj}} p_j \). (In this paragraph, there is no implied sum over the repeated index \( j \), although the sum remains for other Roman indices.) The exponential in the Fourier transform becomes \( e^{i\vec{p}_j\vec{x}_j} \), with \( \vec{x}_j = x_j/\sqrt{K_{jj}} \) (no sum). There is also a nontrivial change in the integration measure,

\[
d^3p = \frac{d^3\vec{p}}{\sqrt{\det K}}.
\]

(39)

bringing the wave function into the form

\[
\psi_0(0, \vec{x}) = \frac{1}{\sqrt{2(\det K)(2\pi)^3/2}} \int d^3\vec{p} \frac{e^{i\vec{p}_{\vec{x}} \vec{x}_j}}{(p_j \bar{p}_j + \mu^2)^{1/4}}.
\]

(40)

From this point, the calculation mirrors the one in the Lorentz-invariant theory. The Fourier transform may be expressed in terms of a Hankel function of fractional order,

\[
\psi_0(0, \vec{x}) = \frac{N}{\sqrt{\det K}} \left( \frac{\mu}{\bar{r}} \right)^{5/4} H_{5/4}(i\mu\bar{r}),
\]

(41)

where the spatial dependence is contained in

\[
\bar{r} = \sqrt{\vec{x}_j \vec{x}_j} = \sqrt{(K^{-1})_{jl}x_j x_l} \approx |\vec{x}| + \frac{k_{jl} x_j x_l}{2|\vec{x}|}
\]

(42)
(with once again a sum over \( j = 1, 2, 3 \)), and \( \mathcal{N} \) is an overall constant. The approximate form in (42) makes use of the fact that \((K^{-1})_{jl} \approx \delta_{jl} + k_{jl} / k \) at leading order in \( k \), in which case \( \sqrt{\det K} \approx 1 - k_{jj} / 2 \) also. For a wave function localized at a different point \( x_0 \), the wave function \( \psi_{\delta 0} (0, \vec{x}) \) still takes the form (41) but with the natural replacement

\[
\vec{r} = \sqrt{(K^{-1})_{ji}(x - x_0)_{i}(x - x_0)_j}.
\]

Because the argument of the Hankel function of the first kind is purely imaginary, the spatial wave function falls off exponentially at large distances, with a characteristic spatial extent \( \sim 1/\mu \). However, it cannot be normalized, since it diverges as \( \vec{r}^{-5/2} \) as \( \vec{r} \to 0 \). (The power law prefactor and the Hankel function each separately go as \( \vec{r}^{-5/4} \) at small \( \vec{r} \).) Qualitatively, the problems with normalizability are quite similar to what is normally encountered with \( \delta \)-function-localized states; there are no issues at long distances, but the divergence in the immediate vicinity of the point of localization makes the states not square integrable. The reason that \( \psi_{\delta 0} (0, \vec{x}) \) cannot be an actual \( \delta \)-function is essentially that the state has to be built entirely out of positive-energy solutions of the Klein–Gordon equation, and the corresponding Hilbert space \( \mathcal{H}_+ \) is not rich enough to represent \( \delta \)-functions. (Something similar may be familiar from the first-quantized Dirac theory, where it is also impossible to construct very narrowly localized wave functions without including negative-energy states.)

Concluding our analysis of the position operator and its eigenstates, we may look at the commutators of the position projections \( x_j^{\text{op}} \) with other important operators. It is apparent from inspection that \( x_j^{\text{op}} \) forms the usual canonical commutation relations with the momenta \( p_i \),

\[
\left[ x_j^{\text{op}}, p_i \right] = i \delta_{ij}.
\]

It is also straightforward that

\[
\left[ x_j^{\text{op}}, x_l^{\text{op}} \right] = 0,
\]

since the second term on the right-hand side of (31) is already proportional to \( \partial / \partial p_j \) acting on \( 1 / p_0 \). According to the Schrödinger Eq. (16), the momentum is still a constant of the motion—no surprise for a free theory. However, the commutator of the Hamiltonian and the position operator is nontrivial,

\[
x_j^{\text{op}} = i \left[ H, x_j^{\text{op}} \right] = i \left[ p_0, x_j^{\text{op}} \right] = \frac{p_j - k_{jl} p_{l}^j}{\mu^2 + \vec{p}^2 - k_{lm} p_l p_m}.
\]

This velocity has the same form as that found for a Lorentz-violating fermion in a theory with \( c \) terms [35]. Moreover, it is also clearly identical to the group velocity \( \vec{v}_g = \nabla \bar{p} / \bar{p} p_0 \).

5 Conclusions and outlook

It is evident that the first-quantized Klein–Gordon theory with Lorentz violation has a number of peculiar features. Some of these are present even in the Lorentz-invariant theory. The necessity of excluding negative-energy states from the theory leads to explicit dependences of many of the theory’s structures—including the inner product in momentum space, the closure relation, and the position operator—on the energy \( p_0 \). With the inclusion of Lorentz violation, the Hamiltonian for the theory is modified, and the Lorentz-violating structure appears in all those energy-dependent structures. This provides a new kind of Lorentz-violating test theory that may be useful for understanding the evolution of spinless particle states.

The theory discussed in this paper sits in an intermediate position between purely classical theories and interacting quantum field theories. Unlike the point-particle Lagrangian theories discussed in Sect. 2, the first-quantized theory is described by a Hilbert space of states and an algebra of operators acting on those states. However, like theories with classical Lagrangians that give only the Lorentz-violating dispersion relations for particle excitations, this Lorentz-violating Klein–Gordon theory is limited to treating only freely propagating excitations. Yet knowledge of how freely-propagating particles with Lorentz-violating dispersion relations behave, on its own, be very powerful. For example, changes to reaction kinematics are often the most important determiners of how Lorentz violation affects particle scattering and decay processes [38, 39]. Up to now, there has also been relatively little examination [35] of how wave packet behavior may be affected by the SME’s anisotropic kinetic energy terms, and the Klein–Gordon theory, which has a complete probabilistic interpretation, provides a new arena for such studies.

Other further examinations of Lorentz-violating Klein–Gordon solutions are also possible. The relationships between the Finsler structure associated with the wave Eq. (12) and the metric of a gravitationally nontrivial spacetime may be made more precise. Moreover, there are remaining questions about the Lorentz-violating Klein–Gordon theory with nonstandard time derivatives, entering via nonzero \( k^{ij} \) terms. Such terms are odd under time reversal and will, at a minimum, affect the separation of positive- and negative-energy modes.

More generally, when considering the possibility of a major change in how physics is understood to operate—and a fundamental violation of Lorentz symmetry would certainly constitute such a basic change—it may be worthwhile to understand the impact of the change from multiple viewpoints. The theories that we use to describe physics—both putatively fundamental theories and
effective ones—may generally be described mathematically in more than one way, meaning via more than just a single formalism. When generalizing such theories, it is not necessarily the case that the modified theories will be describable using all the formalisms that worked for the original theories. That makes it worthwhile to study new physics using more than one mathematical approach, and—like the application of Finsler Lagrangians for classical point particles—the first-quantized Klein–Gordon formalism provides a potentially useful alternative viewpoint for understanding Lorentz violation among bosons.

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