A GENTLE INTRODUCTION TO NEUTRINO OSCILLATIONS

Lecture 4: Relativistic quantum mechanics

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Contents

Chapter 1

RELATIVISTIC QUANTUM MECHANICS

In the preceding chapter we discussed a common approach that represents neutrino mass states by plane waves with fixed momentum and energy. These plane waves have infinite extension in space, which does not seem realistic. A better theory should represent neutrinos by wave packets, which are localized in both position and momentum spaces while conforming with the Heisenberg uncertainty principle. The centers of such wave packets move along well defined trajectories, so that we can talk about particle propagation between the source and the detector. Moreover, owing to the super-relativistic nature of neutrinos, we would like to make this description consistent with the principle of relativity. How can we make our theory relativistically invariant? What does it mean for a quantum theory to be relativistically invariant?

1.1 Poincaré Lie algebra

Operators of momentum P and energy H have a special status: they are *generators of inertial transformations*. For example, if $|\Psi\rangle$ is a state vector from the point of view of observer O, then observer O' shifted in space with respect to O will describe the same state by the vector[1]

[1] Here we use Schrödinger representation of quantum mechanics in which inertial transformations are applied to states, and operators of observables remain unchanged.

$$|\Psi(a)\rangle = e^{iPa/\hbar}|\Psi\rangle, \tag{1.1}$$

where a is the distance of the shift. Time evolution may be regarded as another example of inertial transformation in which the other observer O' is shifted in time with respect to the original one O. Time evolution of the state vector $|\Psi\rangle$ is given by formula

$$|\Psi(t)\rangle = e^{-iHt/\hbar}|\Psi\rangle. \tag{1.2}$$

Hermitian operators P and H appear in arguments of the imaginary exponents in (1.1) - (1.2). This is why they are called generators.

Space and time translations are parts of a larger *group* of inertial transformations, i.e., transformations that change one inertial observer to another inertial (and therefore equivalent) observer.[2] In our 1D space we should also consider inertial transformations of *boosts* or transitions to moving reference frames. Boost generator K is referred to as the *boost momentum*.[3] The action of a boost on a state vector is

$$|\Psi(\theta)\rangle = e^{-iKc\theta/\hbar}|\Psi\rangle \tag{1.3}$$

where parameter $-\infty < \theta < \infty$ is related to the boost velocity by formula

$$v = c\tanh\theta \tag{1.4}$$

Observation: **Inertial transformations form a continuous group (a.k.a. Lie group). Generators P, H, K are called infinitesimal group elements. A theorem can be proven that they form a basis of so-called Lie algebra. In a Lie algebra, a commutator of two generators is equal to a linear combination of generators. All 3D Lie algebras were classified by mathematicians, and there is only one**

[2]It is important to note that any complete set of symmetry transformations forms a mathematical group.

[3]By itself, the boost momentum does not correspond to any common observable, but it is related to the operator of position (1.9).

such algebra whose commutators agree with observations. This is the Poincaré Lie algebra:

$$[H, P] = 0, \tag{1.5}$$
$$[K, H] = -i\hbar P, \tag{1.6}$$
$$[K, P] = -\frac{i\hbar}{c^2} H, \tag{1.7}$$

Wigner's postulate of relativistic invariance: **Each relativistic quantum system is described by a Hilbert space where three symmetry generators P, H, K act as Hermitian operators and satisfy commutation relations (1.5) - (1.6).**

Wigner's postulate says that if we want to build a relativistic quantum theory in a Hilbert space $\mathcal{H}$, our first concern should be construction of the three operators P, H, K with commutation relations (1.5) - (1.7). After this is done, we can find out how finite inertial transformations (1.1) - (1.3) act in our Hilbert space. Moreover, we will be able to define important operators of mass M, center-of-mass position R [1], center-of-mass velocity V

$$M \equiv c^{-2}\sqrt{H^2 - P^2c^2}, \tag{1.8}$$
$$R = -\frac{c^2}{2}(KH^{-1} + H^{-1}K), \tag{1.9}$$
$$V = Pc^2/H, \tag{1.10}$$

and many others. They are built as functions of the generators P, H, K.

Instead of proving Poincaré commutators (1.5) - (1.6), I am going to give some intuitive arguments to make them look more plausible.

Eq. (1.5) tells that space translations and time translations are commutative. This is illustrated in Fig. 1.1. On the left hand side, I apply two consecutive inertial transformations to the hourglass: First, I shift this object to the right,[4] then I apply time translation, i.e., simply wait for a while until all sand drops to the bottom portion. On the right hand side of the figure, the same transformations are performed in reverse order: first

[4] In my arguments I apply inertial transformations directly to the object, i.e., I use *active* form of transformations. Perhaps, it would be more consistent to apply *passive* transformations to the observer. But luckily, these two approaches are equivalent.

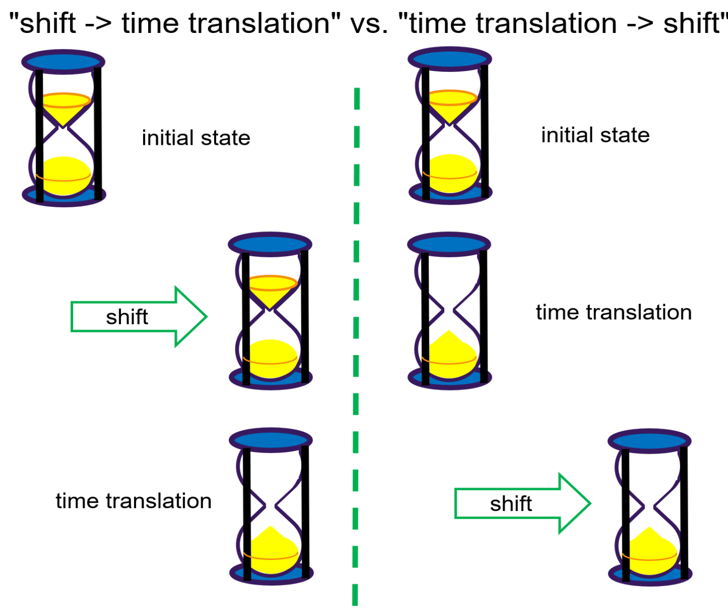

Figure 1.1: Space and time translations are commutative. This implies $[H, P] = 0$.

time translation, then space translation. Obviously, both variants lead to the same final result. This should convince us that space and time translations commute, hence infinitesimal space and time translations should commute as well, which is expressed by eq. (1.5).

In Fig. 1.2, I performed a similar exercise with time translation and boost. Let us imagine a standing car, as shown in the upper left corner of Fig. 1.2. First, I applied a boost transformation by pressing the accelerator pedal. Then, after time translation the car moved a certain distance to the right. On the right hand side of this figure, I applied the same transformations in reverse order. Initially, the car was not moving, so time translation did not do anything to it. Then boost increased car's speed. Obviously, the results of these two pairs of transformations are different. The car on the left is shifted in space with respect to the car on the right. We may conclude that boosts and time translations are not commutative. This fact is expressed by the non-zero commutator of the corresponding generators (1.6).

By applying similar arguments to the pair "boost" + "space translation" we might conclude that they are commutative. But in fact, this conclusion is valid only approximately, i.e., in the non-relativistic world. Indeed, in

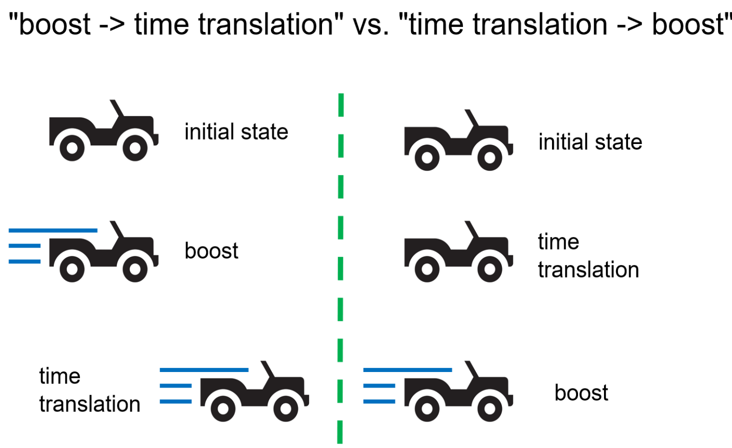

Figure 1.2: Boosts and time translations are not commutative. This implies $[K, H] \neq 0$.

the limit $c \to \infty$ the commutator (1.7) tends to zero.[5] However, in a full relativistic theory boosts and space translations do not commute.

It is remarkable that Wigner's theory relationships (1.1) - (1.10) apply to all physical systems without exception. The only requirement is that this must be an isolated system. Another remarkable thing is that conservation laws are embedded into this formalism quite naturally. Switching for a moment to the Heisenberg representation, we can obtain that the total momentum operator does not depend on time

$$P(t) = e^{iHt/\hbar} P e^{-iHt/\hbar} = P, \tag{1.11}$$

where the last equality follows from the commutator (1.5). Likewise, from the trivial commutator $[H, H] = 0$ it follows that the total energy of any physical system is conserved. A bit more efforts are required to prove that the center of mass of any physical system moves with a constant velocity

[5] This is characteristic for the Galilei Lie algebra, which is a non-relativistic limit of the Poincaré Lie algebra.

$$R(t) = e^{iHt/\hbar} R e^{-iHt/\hbar} = -\frac{c^2}{2} e^{iHt/\hbar}(KH^{-1} + H^{-1}K)e^{-iHt/\hbar} \tag{1.12}$$

$$= R - c^2 t \left(\frac{i}{\hbar}\right) H^{-1}[H, K] = R - c^2 t \left(\frac{i}{\hbar}\right) H^{-1} i\hbar P \tag{1.13}$$

$$= R + \frac{Pc^2 t}{H} = R + Vt \tag{1.14}$$

1.2 Wigner's theory of one particle

Let us apply the above considerations to one massive particle described by momentum-space wave functions $\psi(p)$. We already know expressions for Hermitian generators of space and time translations. They act on particle wave function as follows[6]

$$\hat{P}\psi(p) = p\psi(p) \tag{1.15}$$

$$\hat{H}\psi(p) = \sqrt{m^2c^4 + p^2c^2}\,\psi(p) \tag{1.16}$$

Obviously, these generators commute with each other in agreement with our requirement (1.5).

To make sure that the theory is relativistically invariant, we have to produce the operator of boost K, such that commutators (1.6) - (1.7) are also satisfied. The answer is

$$\hat{K}\psi(p) = -i\hbar \left(\frac{E(p)}{c^2} \frac{d}{dp} + \frac{p}{2E(p)} \right) \psi(p), \tag{1.17}$$

where we denoted

$$E(p) \equiv \sqrt{m^2c^4 + p^2c^2}. \tag{1.18}$$

Now it is not difficult to verify the required commutators. For example, derivation of (1.6) goes as follows

[6] We will place a "hat" above operators when we are interested in their action on wave functions rather than on abstract vectors in the Hilbert space.

$$\begin{aligned}
&\frac{ic^2}{\hbar}[\hat{K},\hat{P}]\psi(p) \\
&= \left[\left(E(p)\frac{d}{dp}+\frac{pc^2}{2E(p)}\right)p - p\left(E(p)\frac{d}{dp}+\frac{pc^2}{2E(p)}\right)\right]\psi(p) \\
&= E(p)p\frac{d\psi(p)}{dp} + E(p)\psi(p) + \frac{p^2c^2}{2E(p)}\psi(p) - E(p)p\frac{d\psi(p)}{dp} - \frac{p^2c^2}{2E(p)}\psi(p) \\
&= E(p)\psi(p) \\
&= \hat{H}\psi(p). \qquad (1.19)
\end{aligned}$$

Particle position is expressed by the operator of differentiation

$$\hat{R} \equiv -\frac{c^2}{2}(\hat{K}\hat{H}^{-1} + \hat{H}^{-1}\hat{K}) = i\hbar\frac{d}{dp}. \qquad (1.20)$$

Position eigenvalues may be interpreted as space coordinates. They form a continuous spectrum that extends from $-\infty$ to $+\infty$. Therefore, we can represent our states as (position-space) wave functions $\psi(r)$ on this spectrum.

In section **??** we already established that position-space wavefunction $\psi(r)$ and momentum-space wavefunction $\psi(p)$ of the same state are related to each other by direct and inverse Fourier transforms

$$\psi(p) = \frac{1}{\sqrt{2\pi\hbar}}\int \psi(r)e^{-ipr/\hbar}dr \qquad (1.21)$$

$$\psi(r) = \frac{1}{\sqrt{2\pi\hbar}}\int \psi(p)e^{ipr/\hbar}dp \qquad (1.22)$$

1.3 Finite inertial transformations. Space translations

It is not difficult to write down finite unitary transformations generated by Hermitian operators (1.15) - (1.17). The action of finite space translation on the momentum space wave function is

$$e^{i\hat{P}a/\hbar}\psi(p) = e^{ipa/\hbar}\psi(p) \qquad (1.23)$$

In the position space, space translation just shifts the wave function argument. This can be verified by applying the Fourier transform (1.22)

$$\begin{aligned} e^{i\hat{P}a/\hbar}\psi(r) &= \frac{1}{\sqrt{2\pi\hbar}} \int e^{ipr/\hbar} \left(e^{ipa/\hbar}\psi(p)\right) dp \\ &= \frac{1}{\sqrt{2\pi\hbar}} \int \psi(p) e^{ip(r+a)/\hbar} dp \\ &= \psi(r+a) \end{aligned} \quad (1.24)$$

1.4 Finite inertial transformations. Time translations

Time translation multiplies momentum-space wave function by a phase factor

$$e^{-i\hat{H}t/\hbar}\psi(p) = e^{-i\sqrt{m^2c^4+p^2c^2}t/\hbar}\psi(p). \quad (1.25)$$

Time evolution in the position space is obtained by Fourier transform

$$\psi(r,t) = e^{-i\hat{H}t/\hbar}\psi(r) = \frac{1}{\sqrt{2\pi\hbar}} \int e^{ipr/\hbar} \left(e^{-i\sqrt{m^2c^4+p^2c^2}t/\hbar}\psi(p)\right) dp. \quad (1.26)$$

Integral (1.26) cannot be calculated analytically, but Hegerfeldt proved the following theorem [2, 3]: *If $\psi(r)$ is initially localized in a bounded region of space, then even after infinitesimally small time the probability of finding the particle anywhere in space becomes non-zero.* This means that the wave packet spreads instantaneously. Immediately after its release the particle has a small but non-zero probability to be found on the Moon.

This conclusion can be illustrated by numerical calculations [4]. For example, Fig. 1.3(a) shows the initial probability density $\rho(r,0) = |\psi(r)|^2$ which was chosen to be of a rectangular shape. Fig. 1.3(b) shows the probability density at a later time t.[7] According to special relativity, the particle is not allowed to move faster than light, therefore its wave packet must be contained between the two vertical broken lines. However, in agreement with

[7] Wave function singularities are not important. They are artifacts of our choice of a non-smooth initial state.

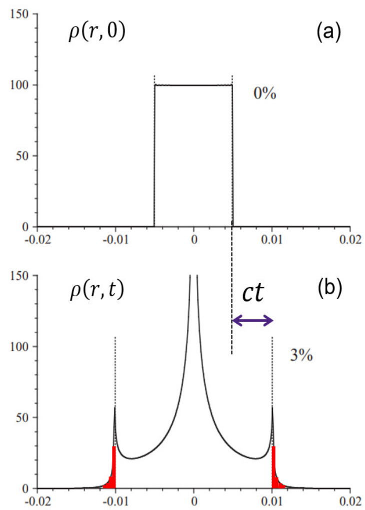

Figure 1.3: Superluminal spreading of one-particle probability density in position-space: (a) initial rectangular wave packet at $t = 0$; (b) the same wave packet at a later time $t > 0$; red colored parts of the wave packet are "leaked" outside the light cone. From Ref. [4].

Hegerfeldt's theorem, there are exponential "tails" extending beyond the light cone. They are shown by red color in Fig. 1.3(b). In the particular case depicted there, the probability for finding the particle outside the light cone is 3 %.

Arguably, there is nothing wrong in the faster-than-light propagation by itself. The true problem emerges when we try to use Lorentz transformations of special relativity to check how this situation looks from the point of view of a moving observer. If the superluminal spreading is allowed, then there is a possibility that events of particle preparation P and detection/measurement M are separated by a space-like interval, as shown in Fig. 1.4(a). Let us now transform these two events to a moving reference frame by using Lorentz formulas of special relativity

$$ct' = ct \cosh\theta - r \sinh\theta, \tag{1.27}$$

$$r' = -ct \sinh\theta + r \cosh\theta. \tag{1.28}$$

Then, for high enough velocity, we will get a situation in which particle detection (point M) occurs earlier than particle preparation (point P). One of

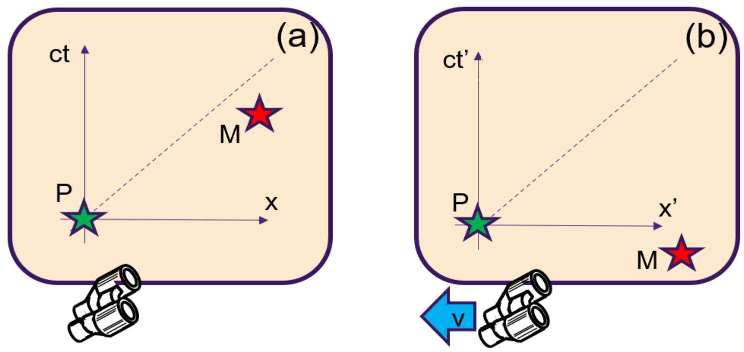

Figure 1.4: Two space-separated events with a cause-effect relationship: particle preparation P and particle measurement M: (a) Superluminal wave packet spreading implies that point M may be outside the light cone w.r.t. point P; (b) According to Lorentz transforms (1.27) - (1.28), a fast moving observer may see that particle is detected *before* being produced. This violates the principle of causality.

the most fundamental ideas in physics is the *principle of causality*, which says that the effect must happen after the cause in all circumstances. Apparently, this important principle gets violated from the point of view of the moving observer. This should not be allowed to happen.

There were dozens of papers written about the causality-violating wave packet spreading. Majority of these works converge on the idea that this problem cannot be solved within traditional quantum mechanics. The prevailing opinion is that relativistic physics is not compatible with such basic quantum-mechanical notions as particles and their wave functions. These ideas should be abandoned and replaced with quantum field theory, where particles emerge only as non-interacting asymptotic states.

Here are some quotes from articles in mainstream journals denouncing the idea of particles.

> *"...it is impossible to prepare a one-particle state which is strictly localized in a given finite space region V."* G. C. Hegerfeldt, Remark on causality and particle localization. Phys. Rev. D 10 (1974) 3320.

> *"...strictly speaking, our talk about localizable particles is a fiction."* H. Halvorson and R. Clifton, No place for particles in

relativistic quantum theories?, Phil. Sci. 69, 1 (2002).

"...there can be no particles in any theory obeying both S[pecial]R[elativity] and quantum physics." A. Hobson, There are no particles, there are only fields. Am. J. Phys. 81, 211 (2013).

In fact, the title of the last article *"There are no particles, there are only fields."* is a good summary of the consensus opinion among majority of theoreticians working in this field.

1.5 Finite inertial transformations. Boosts

If the consensus about the "causality paradox" were correct, then our wave packet approach would become meaningless. However, I would like to argue that the situation is not as hopeless as it looks and that we can continue to use the ideas of particles, wave functions, etc. familiar to us from non-relativistic quantum mechanics.

So far we discussed how particle position-space wave function transforms under space translation (1.24) and time translation (1.26). Let us now check the action of boost – the third type of inertial transformation. From the form of the boost momentum (1.17) it is not difficult to derive the action of a finite boost transformation on a momentum-space wave function

$$e^{-i\hat{K}c\theta/\hbar}\psi(p) = \sqrt{\frac{E(p)\cosh\theta - pc\sinh\theta}{E(p)}}\psi\left(p\cosh\theta - \frac{E(p)}{c}\sinh\theta\right). \tag{1.29}$$

A detailed derivation of this formula and the proof that the function on the right hand side of (1.29) remains normalized can be found in subsections 5.2.2 - 5.2.3 in [5].

The action of boost in the position space can be obtained, as usual, through Fourier integral

$$\begin{aligned} &e^{-i\hat{K}c\theta/\hbar}\psi(r) \\ &= \frac{1}{\sqrt{2\pi\hbar}}\int\left[\sqrt{\frac{E(p)\cosh\theta - pc\sinh\theta}{E(p)}}\psi\left(p\cosh\theta - \frac{E(p)}{c}\sinh\theta\right)\right]e^{ipr/\hbar}dp. \end{aligned} \tag{1.30}$$

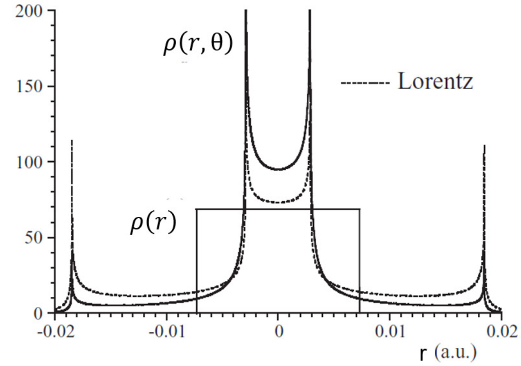

Figure 1.5: Position-space rectangular wave packet viewed from a moving reference frame. Transformation by means of Lorentz formulas (1.27) - (1.28) is also shown by broken line. [4].

Generally, this integral cannot be calculated analytically. However, similar to Hegerfeldt's theorem about time translations, one can prove that if $\psi(r)$ is bounded within a finite region of space, then for any nonzero θ function $\psi(r, \theta)$ extends to spatial infinity $r \to \pm\infty$. With the help of numerical simulation this behavior is demonstrated in Fig. 1.5. The initial probability density $\rho(r) = |\psi(r)|^2$ is chosen to be rectangular, i.e., a non-zero constant in the interval $[-0.007, 0.007]$ (in atomic units) and zero outside this interval. For a moving observer, the probability distribution $\rho(r, \theta) = |\psi(r, \theta)|^2$ spreads out (1.30), and it is important that this wave function has exponential tails that remain non-zero all the way to infinite r.

Taking this result into account, now we can have a fresh look at the causality paradox depicted in Fig. 1.4. In our original discussion we assumed that the particle was prepared in a localized state near the origin $r = 0$ at time $t = 0$. But this statement was true only from the point of view of the rest observer O. According to (1.30), for the moving observer O' the particle loses its localization. This observer does not think that there is a causality paradox, because from his point of view the particle was not prepared initially in a localized state. Even at time $t = 0$, there was a non-zero probability to find the particle on the Moon, so O' does not agree that the particle "propagated" (superluminally or otherwise) from the Earth to the Moon. The particle was always on the Moon, albeit with a low probability. In relativistic quantum mechanics, particle localization is a relative thing. This might be an unusual and troublesome conclusion, but it makes the "causality paradox" to go away.

Conclusion: **The causality paradox has not been proven beyond reasonable doubt. So, for the rest of this work we will continue to use ordinary quantum mechanics with particle wave functions and observables-operators.**

One remarkable consequence of (1.30) is that boost transformation of a position-space wave function can not be done by applying Lorentz transformations (1.27) - (1.28) to function arguments. For example, we are not allowed to write

$$e^{-i\hat{K}c\theta/\hbar}\psi(r,t) = \psi'(r',t') = \psi(r\cosh\theta - tc\sinh\theta, t\cosh/\theta - (r/c)\sinh\theta). \quad (1.31)$$

Such a transformation would lead to an incorrect result as shown by broken line in Fig. 1.5).[8]

One can find more discussion on superluminal spreading and causality in section 8.1 of [7].

[8]Nevertheless, transformations like (1.31) are often regarded as legitimate. For example, it was used in section 2.2 of [6] to "prove" the relativistic invariance of Dirac equation. Transformation (1.31) and Dirac equation make sense when applied to quantum fields, but they are not applicable to wave functions.

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