

NOTATION FOR RELATIVISTIC QUANTUM MECHANICS

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Reference: W. Greiner: *Relativistic Quantum Mechanics (Wave Equations)*; 3rd Edition, Springer-Verlag (2000); Section 1.1.

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Before delving into the main substance of relativistic quantum mechanics, we need to summarize the notation used in Greiner's book.

First, we need to define the term 'relativistic quantum mechanics'. What, exactly, makes an equation 'relativistic'? The central point is that a relativistic quantum mechanical wave equation needs to be invariant under Lorentz transformations. That is, if a wave equation describes a system in one inertial frame, then the equation must have the same form when used by an observer in another inertial frame moving at constant velocity relative to the first frame. Since special relativity treats time and space coordinates on an equal footing, any wave equation must also treat time and space equally. The Schrödinger equation doesn't do this, since time appears as a first derivative while the three spatial coordinates appear as second derivatives:

$$i\hbar \frac{\partial \Psi}{\partial t} = -\frac{\hbar^2}{2m} \nabla^2 \Psi + V(x, t) \Psi \quad (1)$$

In special relativity, many physical quantities are defined as four-vectors. The four components of a four-vector are indicated with either a superscript or subscript, and the vector itself is usually written in normal font (as opposed to bold face that is usually used for 3-d vectors). Thus a four-vector a has components

$$a = (a_0, a_1, a_2, a_3) \quad (2)$$

The components of a four-vector can exist in two different forms. When the coordinate index is a subscript, the component is said to be *covariant*; when it is a superscript, it is *contravariant*.

Although the difference between covariant and contravariant components can get quite complicated in general relativity, in special relativity the relation between the two forms is fairly simple. To convert from one form to the other we multiply a component by the metric tensor $g_{\mu\nu}$. Unfortunately, there are two different versions of this metric tensor that seem to occur in equal proportions in textbooks. Greiner uses the form

$$g_{\mu\nu} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} \quad (3)$$

Here, the top row and left-most column have index 0, and the index increases as we move to the right or down. With this definition, the relation between covariant and contravariant components is

$$a^0 = a_0 \quad (4)$$

$$a^i = -a_i \quad i = 1, 2, 3 \quad (5)$$

That is, the 0 component is the same for both covariant and contravariant forms, while the other three components change sign. Beware that many other books use the opposite convention, where

$$g_{\mu\nu} = \begin{bmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad (6)$$

With this convention, the 0 component changes sign while the other three do not.

The metric tensor can be used to raise or lower an index on a four-vector, so we have

$$a_\mu = g_{\mu\nu} a^\nu \quad (7)$$

This equation uses the Einstein summation convention, where a repeated Greek index such as μ in a product is summed from 0 to 3. (A repeated Roman index such as i is summed from 1 to 3.) We can see that this equation does indeed give the behaviour in 5.

The metric tensor itself can have its indices raised or lowered using the same formula. Raising or lowering the 0 index leaves things unchanged, while raising or lowering the index $i = 1, 2, 3$ changes the sign. So we have

$$g^\mu_\nu = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} = \delta^\mu_\nu \quad (8)$$

$$g^{\mu\nu} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{bmatrix} = g_{\mu\nu} \quad (9)$$

The scalar product of two four-vectors produces a scalar, which is a quantity that is invariant under a Lorentz transformation. Unlike the traditional scalar or dot product for 3-d vectors, however, the scalar product of two four-vectors is defined as

$$ab = a^\mu b_\mu \equiv \sum_{\mu=0}^3 a^\mu b_\mu \quad (10)$$

$$= g^{\mu\nu} a_\mu b_\nu \quad (11)$$

$$= a_0 b_0 - a_1 b_1 - a_2 b_2 - a_3 b_3 \quad (12)$$

Some special four-vectors commonly found in RQM are the space-time vector and the energy-momentum vector. The definitions used by Greiner are

$$x_\mu = \{ct, -x, -y, -z\} \quad (13)$$

$$p_\mu = \left\{ \frac{E}{c}, -p_x, -p_y, -p_z \right\} \quad (14)$$

By applying the metric tensor, we can get the contravariant components as

$$x^\mu = g^{\mu\nu} x_\nu = \{ct, x, y, z\} \quad (15)$$

$$p^\mu = g^{\mu\nu} p_\nu = \left\{ \frac{E}{c}, p_x, p_y, p_z \right\} \quad (16)$$

These two vectors can be used to form the relativistic invariant quantities

$$x \cdot x = x^\mu x_\mu = c^2 t^2 - \mathbf{x} \cdot \mathbf{x} \quad (17)$$

$$p \cdot p = p^\mu p_\mu = \frac{E^2}{c^2} - \mathbf{p} \cdot \mathbf{p} \quad (18)$$

In quantum mechanics, the momentum is an operator:

$$\hat{\mathbf{p}} = -i\hbar\nabla \quad (19)$$

In the 1, the operator on the LHS generates the energy, so it can be considered as the energy operator. That is

$$\hat{E} = i\hbar \frac{\partial}{\partial t} \quad (20)$$

We can combine these two operators to get a four-vector operator for energy and momentum combined. That is,

$$\hat{p}^\mu = \left\{ \frac{\hat{E}}{c}, \hat{p}^1, \hat{p}^2, \hat{p}^3 \right\} \quad (21)$$

When we use 19 to write this in terms of derivatives, we need to be careful to specify whether we are using covariant or contravariant components for the spatial coordinates. Contravariant and covariant tensors are actually defined by how they transform under a coordinate transformation, and it turns out that the derivative with respect to a contravariant coordinate results in a covariant four-vector, and vice versa. That is, we're justified in writing

$$\hat{p}^\mu = i\hbar \frac{\partial}{\partial x_\mu} \quad (22)$$

or

$$\hat{p}_\mu = i\hbar \frac{\partial}{\partial x^\mu} \quad (23)$$

The quantum operator 19 is, in terms of ordinary 3-d coordinates

$$\hat{\mathbf{p}} = \left[-i\hbar \frac{\partial}{\partial x}, -i\hbar \frac{\partial}{\partial y}, -i\hbar \frac{\partial}{\partial z} \right] \quad (24)$$

When the coordinates are part of a covariant four-vector, we need to use the definition 13, where the spatial coordinates occur as negatives of the 'ordinary' coordinates. Therefore

$$\hat{\mathbf{p}} = \left[i\hbar \frac{\partial}{\partial x_1}, i\hbar \frac{\partial}{\partial x_2}, i\hbar \frac{\partial}{\partial x_3} \right] \quad (25)$$

Notice that we've dropped the minus signs here, since $x_1 = -x$, etc. Putting this together with the energy term, we get

$$\hat{p}^\mu = i\hbar \frac{\partial}{\partial x_\mu} = \left\{ i\hbar \frac{\partial}{\partial(ct)}, i\hbar \frac{\partial}{\partial x_1}, i\hbar \frac{\partial}{\partial x_2}, i\hbar \frac{\partial}{\partial x_3} \right\} \quad (26)$$

$$= \left\{ i\hbar \frac{\partial}{\partial(ct)}, -i\hbar \frac{\partial}{\partial x}, -i\hbar \frac{\partial}{\partial y}, -i\hbar \frac{\partial}{\partial z} \right\} \quad (27)$$

$$= i\hbar \left\{ \frac{\partial}{\partial(ct)}, -\nabla \right\} \quad (28)$$

$$\equiv i\hbar \nabla^\mu \quad (29)$$

We've introduced ∇^μ as a contravariant four-vector operator, which is defined by comparing it with the penultimate line. Note that the spatial component of ∇^μ is the *negative* of the ordinary gradient operator ∇ .

The scalar product of the momentum operator with itself is now

$$\hat{p}^\mu \hat{p}_\mu = -\hbar^2 \nabla^\mu \nabla_\mu \quad (30)$$

$$= -\hbar^2 \frac{\partial}{\partial x_\mu} \frac{\partial}{\partial x^\mu} \quad (31)$$

$$= -\hbar^2 g^{\mu\sigma} \frac{\partial}{\partial x_\sigma} \frac{\partial}{\partial x_\mu} \quad (32)$$

$$= -\hbar^2 \left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} - \frac{\partial^2}{\partial y^2} - \frac{\partial^2}{\partial z^2} \right) \quad (33)$$

$$= -\hbar^2 \left(\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \right) \quad (34)$$

$$\equiv \hbar^2 \square \quad (35)$$

where \square is the d'Alembertian operator

$$\square \equiv \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2 \quad (36)$$

[Note that some books define the d'Alembertian as \square^2 rather than just \square . Also Greiner uses the symbol Δ instead of ∇^2 .]

Finally, the commutation relations can be written as

$$[\hat{p}^\mu, x^\nu] = i\hbar \left[\frac{\partial}{\partial x_\mu}, x^\nu \right] \quad (37)$$

To work out these commutators we can apply the RHS to some function $f(x^\nu)$ (note that f is a function of all four spacetime coordinates, so it is also a function of time). First, we should get the coordinates into the same form, so we have

$$i\hbar \left[\frac{\partial}{\partial x_\mu}, x^\nu \right] = i\hbar \left[\frac{\partial}{\partial x_\mu}, g^{\nu\sigma} x_\sigma \right] \quad (38)$$

We can now apply it to f :

$$\left[\frac{\partial}{\partial x_\mu}, g^{\nu\sigma} x_\sigma \right] f = g^{\nu\sigma} \left[\frac{\partial}{\partial x_\mu} (x_\sigma f) - x_\sigma \frac{\partial f}{\partial x_\mu} \right] \quad (39)$$

$$= g^{\nu\sigma} \left[\frac{\partial x_\sigma}{\partial x_\mu} f + x_\sigma \frac{\partial f}{\partial x_\mu} - x_\sigma \frac{\partial f}{\partial x_\mu} \right] \quad (40)$$

$$= g^{\nu\sigma} \frac{\partial x_\sigma}{\partial x_\mu} f \quad (41)$$

Removing f we see that

$$[\hat{p}^\mu, x^\nu] = i\hbar g^{\nu\sigma} \frac{\partial x_\sigma}{\partial x_\mu} \quad (42)$$

Since the coordinates are independent, we have

$$\frac{\partial x_\sigma}{\partial x_\mu} = \delta_\sigma^\mu \quad (43)$$

so we end up with

$$[\hat{p}^\mu, x^\nu] = i\hbar g^{\mu\nu} \quad (44)$$

This is equivalent to the usual commutator for 3-d position and momentum, since if μ and ν are spatial indices, we have

$$[\hat{p}^i, x^j] = -[x^j, \hat{p}^i] = -i\hbar \delta_{ij} \quad (45)$$

However, there is also a commutator involving energy and time, since if $\mu = \nu = 0$ we get

$$[\hat{p}^0, x^0] = \left[\frac{\hat{E}}{c}, ct \right] = [\hat{E}, t] = i\hbar \quad (46)$$

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