# **Quantum Field Theory**

Lecture Notes

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# Preface

Should authors feel compelled to justify the writing of yet another lecture notes on Quantum Field Theory? In an overpopulated world, should parents feel compelled to justify bringing forth yet another child? Perhaps not! But an act of creation is also an act of love, and a love story can always be happily shared. These notes originated from a series of lectures on Quantum Filed Theory delivered at the Faculty of Nuclear Science and Physical Engineering, Czech Technical University in Prague, over the period from 2019 to 2020. During the writing, I have attempted to maintain a cohesive self-contained content. The material is discussed in sufficient detail to enable the students to follow every step, but some crucial theoretical aspects are not covered such as the non-perturbative aspects of Yang–Mills gauge theories or quantum field theory of gravity. Still it is hoped that these notes will serve as a useful introduction to Quantum Field Theory.

A working knowledge of basic quantum mechanics and related mathematical formalisms, e.g., Hilbert spaces and operators, is required to understand the contents of these lecture notes. Nevertheless, I have attempted to recall necessary definitions throughout the chapters and the numerous notes.

I would like to express my gratitude to Doctors V. Zatloukal and J. Kňap for their diligent reading of the manuscript and constructive criticisms. Also special thanks go to M. Blasone, G. Vitiello and H. Kleinert for teaching me non-perturbative techniques, as well as to the students of QFT I and II courses for their patience and their numerous suggestions. Finally these notes would not have seen the light of day had it not been for the heroic efforts of three modern day scribes and illuminators, Georgy Ponimatkin, David Grund and Diana Mária Krupová to whom I am deeply grateful.

## Books

There are many books on Quantum Field Theory, most are rather long. All those listed below are worth looking at. They provide a wealth of a complemental material for these lecture notes.

► E.M. Peskin and D.V Schroeder, *An Introduction to Quantum Field Theory*, (Addison-Wesley Publishing Co., 1996).

Provides a good introduction with an extensive discussion of gauge theories

including QCD and various applications.

- ► M. Srednicky, *Quantum Field Theory*, (Cambridge University Press, 2007). Represents a comprehensive modern book organised by considering spin-0, spin-1 2 and spin-1 fields in turn.
- S. Weinberg, *The Quantum Theory of Fields, vol. I Foundations* and *vol. II Modern Applications*, (Cambridge University Press, 1995,1996).
   Written by a Nobel Laureate, contains lots of details which are not covered elsewhere, perhaps a little idiosyncratic and less introductory than the above.
- Z. Zinn-Justin, Quantum Field Theory and Critical Phenomenam, (Oxford University Press, 2002).
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Book devotes a large fraction to applications to critical phenomena in statistical physics but covers gauge theories at some length as well, not really an introductory book.

► C. Itzykson and J.-B. Zuber, *Quantum Field Theory*, (McGraw-Hill International Book Co., 1980).

At one time the standard book, containing a lot of detailed calculations but the treatment of non abelian gauge theories is a bit cursory and somewhat dated.

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# Relativistic Quantum Mechanics

# 1

# 1.1 Relativistic Conventions

Here and throughout we will assume so-called *natural units*, in which  $c = \hbar = 1$ . In this system of units, *E*, *p* have units of lenght<sup>-1</sup> = time<sup>-1</sup>. So, as for their units *time* and *space* are considered on equal footing.

Also the following relativistic conventions are used:

- Space-time 4-vector will be denoted by  $x^{\mu} = (x^0, \mathbf{x}) = (t, \mathbf{x})$ .
- ▶ 4-momentum will be denoted by  $p^{\mu} = (p^0, p) = (E, p)$ .
- ► Scalar product is given by

$$a \cdot b = g_{\mu\nu} a^{\mu} b^{\nu} = a^{\mu} b_{\mu} = a_{\mu} b^{\mu} , \qquad (1.1)$$

where

$$\boldsymbol{g}_{\mu\nu} = \boldsymbol{g}^{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \operatorname{diag}(1, -1, -1, -1), \quad (1.2)$$

is a metric tensor, with  $g^{\mu\nu}$  being inverse to the  $g_{\mu\nu}$ . We can immediately derive a simple relation between metric tensors and Kronecker delta:

$$\boldsymbol{g}_{\mu\nu}\boldsymbol{g}^{\nu\sigma} = \delta_{\mu}^{\ \sigma} \,. \tag{1.3}$$

A *Lorentz transformation L* maps 4-vectors according to the linear relation

$$x^{\mu} \stackrel{L}{\to} x^{\prime \mu} = L^{\mu}_{\ \nu} x^{\nu}. \tag{1.4}$$

Here  $L^{\mu}_{\nu} \in SO(1,3)$  is element of the so-called *Lorentz group*. If we define the inverse transform as

$$x^{\nu} = L_{\mu}^{\ \nu} x^{\prime \mu} , \qquad (1.5)$$

we see that  $L_{\mu}^{\nu}$  and  $L_{\nu}^{\mu}$  are inverse to each other. From the fact that Lorentz transformation should preserve scalar product of 4-vectors, i.e.  $a' \cdot b' = a \cdot b$ , the following relations must hold

$$g^{\mu\mu'}L^{\nu}{}_{\mu}L^{\nu'}{}_{\mu'} = g^{\nu\nu'}, \qquad (1.6)$$

$$g^{\mu\mu'}L_{\mu}^{\nu}L_{\mu'}^{\nu'} = g^{\nu\nu'}. \qquad (1.7)$$

By taking determinant of both sides of (1.6) we arrive at the fact that

$$\det^2 L = 1. (1.8)$$

Hence we can divide Lorentz transformations into two classes — *proper*, for which det L = 1 and *improper*, for which det L = -1.

#### Differentials

We define differential as a scalar operator given by

$$d \equiv dx^{\mu} \frac{\partial}{\partial x^{\mu}} \,. \tag{1.9}$$

In relativistic notation we define  $\partial_{\mu} \equiv \frac{\partial}{\partial x^{\mu}}$ , then differential can be then written as

$$d = dx^{\mu}\partial_{\mu}. \tag{1.10}$$

Such definition of *d* is Lorentz invariant (as can be shown from the fact that  $\partial'_{\mu} = L^{\nu}_{\mu} \partial_{\nu}$ ). We define covariant 4-gradient operator to be

$$\partial_{\mu} = \left(\frac{\partial}{\partial x_0}, \nabla\right),$$
 (1.11)

and its contravariant counterpart as

$$\partial^{\mu} = \left(\frac{\partial}{\partial x_0}, -\nabla\right). \tag{1.12}$$

Using those we can define *d'Alambertian operator* as

$$\mathbf{g}^{\mu\nu}\partial_{\mu}\partial_{\nu} = \partial_{\mu}\partial^{\mu} = \left(\frac{\partial^2}{\partial x_0^2} - \nabla^2\right) \equiv \Box.$$
 (1.13)

In the context of special relativity it is common to denote the metric tensor  $g^{\mu\nu}$  as  $\eta^{\mu\nu}$  or simply  $\eta^{\mu\nu}$ .

## **1.2 Structure of Lorentz Transformation**

We begin our study of Lorentz transformations by taking infinitesimal limit of such transformation

$$L^{\mu}_{\ \nu} = \delta^{\mu}_{\ \nu} + \omega^{\mu}_{\ \nu}, \qquad (1.14)$$

which can be thought of as infinitesimal deformation from identical transformation (here  $||\omega|| \ll 1$ ). Starting from (1.6) and raising indices by metric tensor we get

$$L^{\mu\nu'}L_{\mu}^{\nu} = g^{\nu'\nu}. \qquad (1.15)$$

Then acting on (1.15) with  $g_{\nu\alpha}$  from right we get

$$L^{\mu\nu'}L_{\mu\alpha} = g^{\nu'}{}_{\alpha} = \delta^{\nu'}{}_{\alpha}.$$
(1.16)

This can be equivalently rewritten as

$$L_{\mu}^{\nu'}L_{\alpha}^{\mu} = \delta_{\alpha}^{\nu'}. \tag{1.17}$$

By using (1.14) we finally arrive to the following equation

$$(\delta_{\mu}^{\nu'} + \omega_{\mu}^{\nu'})(\delta^{\mu}_{\ \alpha} + \omega^{\mu}_{\ \alpha}) = \delta^{\nu'}_{\ \alpha}.$$
(1.18)

If we restrict ourselves only to the first order in  $\omega$ 

$$\delta_{\alpha}^{\nu'} + \omega_{\alpha}^{\nu'} + \omega_{\alpha}^{\nu'} = \delta_{\alpha}^{\nu'}.$$
(1.19)

By subtracting Kronecker  $\delta$ 's from both sides and lowering all indices one gets

$$\omega_{\alpha\nu'} + \omega_{\nu'\alpha} = 0. \tag{1.20}$$

This statement implies that  $\omega$  is a 4×4 antisymmetric matrix, which has 6 independent parameters in the case of infinitesimal Lorentz transformation. This fact also holds for finite Lorentz transformations.

#### Properties of Lie groups (some preliminaries)

The transformation laws of continuous groups (Lie groups) such as rotation or Lorentz group are typically conveniently expressed in an infinitesimal form. By combining successive infinitesimal transformations it is always possible to reconstruct from these the finite transformation laws. This is a consequence of the fact that exponential function  $e^x$  can always be obtained by a product of many small-*x* approximations. In particular, consider  $e^{\delta \alpha X} \approx$  $1 + \delta \alpha X$ , where  $\delta \alpha = \alpha/N$ ,  $N \gg 1$ . By taking successive applications of *N* such infinitesimal transformations we obtain

$$(1 + \alpha X/N)(1 + \alpha X/N) \times \ldots \times (1 + \alpha X/N) = (1 + \alpha X/N)^N,$$

which in the limit of large *N* tends to  $e^{\alpha X}$ . This can also be extended to more parameters  $\alpha_i$ . In such a case one should substitute  $\alpha X$  with  $\sum_i \alpha_i X_i$ . Here  $X_i$  are the so-called *group generators*. The finite group transformation is then given by  $L(\alpha) = e^{\sum_i \alpha_i X_i}$ . One can recover the group generators from a generic group element  $L(\alpha)$  by taking  $\frac{\partial L(\alpha)}{\partial \alpha_i}\Big|_{\alpha=0} = X_i$ .

When we pass from infinitesimal to finite transformation, the generic group element will read

$$L^{\rho}_{\ \tau} = \left( e^{-\frac{i}{4}M^{\mu\nu}\omega_{\mu\nu}} \right)^{\rho}_{\ \tau} .$$
 (1.21)

We can find  $M^{\mu\nu}$  by comparing expression (1.21) for  $\|\omega_{\mu\nu}\| \ll 1$  ( $\omega_{\mu\nu} = -\omega_{\nu\mu}$ ) with the infinitesimal form of  $L^{\rho}_{\tau}$  given by (1.14). This yields

$$L^{\rho}{}_{\tau} = \delta^{\rho}{}_{\tau} - \frac{i}{4} (M^{\mu\nu})^{\rho}{}_{\tau} \omega_{\mu\nu} = \delta^{\rho}{}_{\tau} + \omega^{\rho}{}_{\tau}$$
$$= \delta^{\rho}{}_{\tau} + \eta^{\rho\mu} \eta_{\tau}{}^{\nu} \omega_{\mu\nu} = \delta^{\rho}{}_{\tau} + \frac{1}{2} \eta^{\rho\mu} \delta_{\tau}{}^{\nu} (\omega_{\mu\nu} - \omega_{\nu\mu})$$
$$= \delta^{\rho}{}_{\tau} + \frac{1}{2} (\eta^{\rho\mu} \delta^{\nu}{}_{\tau} - \eta^{\rho\nu} \delta^{\mu}{}_{\tau}). \qquad (1.22)$$

From this we have

$$\left(\boldsymbol{M}^{\mu\nu}\right)^{\rho}{}_{\tau} = 2i\left(\eta^{\rho\mu}\delta^{\nu}_{\tau} - \eta^{\rho\nu}\delta^{\mu}_{\tau}\right). \tag{1.23}$$

### **1.3 Relativistic Wave Equations**

A spinless relativistic particle can be described in terms of a scalar wave function  $\phi(\mathbf{x}, t)$ . This wave function can't posses any internal index, which would otherwise bear information about other degrees of freedom, such as spin. Relativistic particles satisfy the energy-momentum dispersion relation

$$E = \sqrt{m^2 + p^2}.$$
 (1.24)

Recall that  $p^{\mu} = (E, \mathbf{p})$  and that there exists a relativistic invariant given by

$$p^{\mu}p_{\mu} = p_0^2 - p^2 = m^2. \qquad (1.25)$$

In the formalism of first quantization, quantum mechanics is brought about by identifying operators with dynamical quantities

$$\boldsymbol{p} \to -i\boldsymbol{\nabla}, \quad E \to i\frac{\partial}{\partial t}.$$
 (1.26)

Applying this prescription to the relativistic invariant (1.25) we arrive at the following equation

$$\left(-\frac{\partial^2}{\partial t^2} + \nabla^2\right)\phi(x) = m^2\phi(x).$$
(1.27)

From the fact that  $\partial_{\mu} = \left(\frac{\partial}{\partial t}, \nabla\right)$  we can equivalently rewrite this equation as

$$\partial^{\mu}\partial_{\mu}\phi = \Box\phi = -m^{2}\phi. \qquad (1.28)$$

Finally, we arrive at the relativistic wave equation known as the Klein–Gordon equation, given by

$$(\Box + m^2)\phi(x) = 0.$$
 (1.29)

If we accept this equation and seek solution of a definite energy and momentum, we get

$$\phi(x) \propto e^{-ipx} = e^{-iEt+i\mathbf{p}\cdot\mathbf{x}} = e^{-ip_0x_0+i\mathbf{p}\cdot\mathbf{x}}.$$
 (1.30)

Adopting  $\partial_{\mu}\phi = -ip_{\mu}\phi$  we get that  $\Box\phi = -p^{2}\phi$  and then

$$(-p^2 + m^2)\phi = 0. (1.31)$$

So if  $\phi \neq 0$  we have condition that  $p^2 = m^2$  and hence

$$E = \pm \sqrt{p^2 + m^2}.$$
 (1.32)

#### Why can't we directly quantize relativistic energy relation?

A question may rise, why can't we directly quantize dispersion relation  $\omega_p = E_p = \sqrt{p^2 + m^2}$  using fact that  $p \rightarrow -i\nabla$ ? To make sense to such a function of operator we have to interpret it in terms

In classical relativity we do not consider negative sign in the dispersion relation.

Klein–Gordon equation just reflects energy dispersion relation (similarly as Schrödinger equation) so, all relativistic wave functions should satisfy this equation.

Both positive and negative energy solutions are relevant in relativistic quantum theory! of the Taylor expansion:

$$H_{p} = \sqrt{p^{2} + m^{2}} = m \left(1 + \frac{p^{2}}{m^{2}}\right)^{\frac{1}{2}} = m + \frac{p^{2}}{2m} - \frac{p^{4}}{8m^{3}} + \cdots$$

Unfortunately, in this way we can not form covariant wave equation, i.e. if we formed a coordinate space representation of a state vector  $|\psi\rangle$ , the resulting wave equation would have *one* time derivative and *infinite* series of increasing spatial derivatives. There is no way to put time and space on an "equal footing". Nonetheless, let us go ahead and try to build a wave equation

$$i \frac{\partial}{\partial t} \langle \mathbf{x} | \psi(t) \rangle = \langle \mathbf{x} | H_{\mathbf{p}} | \psi(t) \rangle.$$

The matrix element  $\langle \mathbf{x} | H_{\mathbf{p}} | \psi(t) \rangle$  is proportional to the infinite sum of  $\langle \mathbf{x} | \mathbf{p}^n | \psi(t) \rangle = (-i)^n \frac{\partial^n}{\partial x^n} \langle \mathbf{x} | \psi(t) \rangle$  terms. This in turn renders wave function to be *non-local*, since it must reach further and further away from the region near  $\mathbf{x}$  in order to evaluate the time derivative. Indeed, while the left-hand side can be written as

$$\lim_{\Delta t \to 0} \frac{\langle \boldsymbol{x} | \boldsymbol{\psi}(t + \Delta t) \rangle - \langle \boldsymbol{x} | \boldsymbol{\psi}(t) \rangle}{\Delta t}$$

a typical term on the right-hand side, i.e., term  $(-i)^n \frac{\partial^n}{\partial x^n} \langle \mathbf{x} | \psi(t) \rangle$  has the form (for simplicity we consider  $\mathbf{x}$  to be one-dimensional)

$$\lim_{\Delta x \to 0} \frac{(-i)^n}{(\Delta x)^n} \sum_{k=0}^n (-1)^k \binom{n}{k} \langle x + \left(\frac{n}{2} - k\right) \Delta x | \psi(t) \rangle \,.$$

So, on the right-hand side we need all possible integer multiples of  $\Delta x$ . Eventually, the causality will be violated for any spatially localized function  $\langle \mathbf{x} | \psi(t) \rangle$  since for understanding physics in the interval  $\Delta t$  we need to know physics in the interval  $\bar{\Delta} x = k \Delta x$  (*k* is an arbitrary integer), which for sufficiently large *k* certainly satisfies  $\Delta x^{\mu} \Delta x_{\mu} = (\Delta x^{0})^{2} - (\bar{\Delta} \mathbf{x})^{2} < 0$ , i.e., we require space-like separated events. Because of that we must abandon this approach and work with square of  $H_{p}$ , (i.e.,  $\omega_{p}^{2}$ ) instead. This will remove the problem of the square root, but will introduce a different problem — negative energies. This will still prove to be more useful way to proceed.

Let us look at non-relativistic limit of Klein–Gordon equation. A mode with  $E = m + \varepsilon$  would oscillate in time as  $\phi \propto e^{-iEt}$ . In the non-relativistic regime  $\varepsilon$  is much smaller than the rest mass *m*. We can factor-out the fast-oscillating part of the  $\phi$  away and rewrite it as

$$\phi(x) = \phi(\mathbf{x}, t) = e^{-imt}\varphi(\mathbf{x}, t).$$
(1.33)

Field  $\varphi$  is oscillating much more slowly that  $e^{-imt}$  in time. By inserting this into the Klein–Gordon equation and using the fact that

$$\frac{\partial}{\partial t}e^{-imt}\varphi(\mathbf{x},t) = e^{-imt}\left(-im + \frac{\partial}{\partial t}\right)\varphi(\mathbf{x},t), \qquad (1.34)$$

Here we use the so-called *central difference relation* for *n*-th derivative. we obtain

$$\left(\frac{\partial}{\partial t} - \nabla^{2} + m^{2}\right)\phi(x)$$

$$= \frac{\partial}{\partial t}\left[e^{-imt}\left(-im + \frac{\partial}{\partial t}\right)\varphi\right] - e^{-imt}\nabla^{2}\varphi(x,t) + m^{2}e^{-imt}\varphi$$

$$= e^{-imt}\left(-im + \frac{\partial}{\partial t}\right)\left(-im + \frac{\partial}{\partial t}\right)\varphi - e^{-imt}\nabla^{2}\varphi + m^{2}e^{-imt}\varphi$$

$$= e^{-imt}\left[\left(-m^{2} - 2im\frac{\partial}{\partial t} + \frac{\partial^{2}}{\partial t^{2}}\right)\varphi - \nabla^{2}\varphi + m^{2}\varphi\right] = 0. \quad (1.35)$$

Dropping  $\frac{\partial^2 \phi}{\partial t^2}$  as small compared to  $-imt \frac{\partial \phi}{\partial t}$  we find that

$$i\frac{\partial}{\partial t}\varphi = -\frac{\nabla^2}{2m}\varphi, \qquad (1.36)$$

which is nothing but the Schrödinger equation for a free particle.

Let us focus on general solution to the Klein-Gordon equation,  $\phi(x)$ . With the help of Fourier decomposition we can write

$$\phi(x) = \int \frac{\mathrm{d}^4 p}{(2\pi)^3} e^{-ipx}$$

To find the solution we will solve the Klein-Gordon equation in momentum space, which yields

$$(p^2 - m^2)\tilde{\phi}(p) = 0.$$
 (1.38)

Equations of this form are solved by the Dirac  $\delta$ -functions. In particular, the solution in momentum space reads

$$\widetilde{\phi}(p) = f(p)\delta(p^2 - m^2)$$

$$= \frac{f(p)\delta(p_0 + \sqrt{p^2 + m^2})}{2\sqrt{p^2 + m^2}} + \frac{f(p)\delta(p_0 - \sqrt{p^2 + m^2})}{2\sqrt{p^2 + m^2}}. (1.39)$$

Using this knowledge and denoting  $\omega_p = \sqrt{p^2 + m^2}$ , we can write the full solution as

$$\phi(x) = \int \frac{d^4p}{(2\pi)^3} \frac{1}{2\omega_p} e^{-ipx} [f(p)\delta(p_0 + \omega_p) + f(p)\delta(p_0 - \omega_p)]$$
  
$$= \int \frac{d^3p}{(2\pi)^3} \frac{1}{2\omega_p} [e^{-i\omega_p t + i\mathbf{p}\cdot\mathbf{x}} f(\omega_p, \mathbf{p}) + e^{i\omega_p t + i\mathbf{p}\cdot\mathbf{x}} f(-\omega_p, \mathbf{p})]$$
  
$$= \int \frac{d^3p}{(2\pi)^3} \frac{1}{2\omega_p} [e^{-ipx} \underbrace{f(\omega_p, \mathbf{p})}_{f(\mathbf{p})} + e^{ipx} \underbrace{f(-\omega_p, -\mathbf{p})}_{g(\mathbf{p})}]. \quad (1.40)$$

Here  $p^{\mu} = (\omega_p, \boldsymbol{p})$ .

So, we see that a general solution of the Klein-Gordon equation is a superposition of positive and negative energy eigenstate solutions.

By the way, the Klein-Gordon equation was actually discovered before Schrödinger equation by Erwin Schrödinger himself.

Here we use the well known property of Dirac  $\delta$ -function, namely that  $\delta(f(x)) =$  $\sum_i \frac{\delta(x-x_i)}{|f'(x_i)|}$ , where  $x_i$  are roots of f.

If we want to interpret  $\phi(x)$  as a wave function, we have to find a nonnegative norm, which is conserved by time evolution and is Lorentz invariant. Let us define the norm of  $\phi(x)$  to be

$$||\phi||^2 = (\phi|\phi) = i \int d^3 \mathbf{x} \left[ \phi^* \frac{\partial \phi}{\partial x^0} - \left( \frac{\partial \phi}{\partial x^0} \right)^* \phi \right].$$
(1.41)

This is, in a sense, a natural candidate for the norm. The naturalness of this choice comes from the analogy with quantum mechanics — continuity equation, which defines the probability density.

We know that each 4-current should have the form  $J_{\mu} = (\rho, J)$  and should be conserved (after equations of the motion are taken into account), i.e.,  $\partial^{\mu}J_{\mu} = 0$ . To this end we consider the 4-current

$$J_{\mu}(x) = \frac{i}{2m} \left[ \phi^* \partial_{\mu} \phi - (\partial_{\mu} \phi)^* \phi \right] , \qquad (1.42)$$

(factor 1/2m is only a convention that ensures a correct non-relativistic limit, see Eq. (1.45)). Eq. (1.42) can be equivalently rewritten as

$$J(x) = \frac{i}{2m} \left[ \phi^* \nabla \phi - (\nabla \phi)^* \phi \right],$$
  

$$\rho(x) = \frac{i}{2m} \left[ \phi^* \partial_0 \phi - (\partial_0 \phi)^* \phi \right].$$
(1.43)

Let us now compute  $\partial_{\mu} J^{\mu}$ :

$$\partial^{\mu} J_{\mu}(x) = i \left[ \partial_{\mu} (\phi^{*} \partial^{\mu} \phi) - \partial_{\mu} (\phi \partial^{\mu} \phi^{*}) \right]$$
  
$$= i \left[ (\partial_{\mu} \phi^{*}) (\partial^{\mu} \phi) + \underbrace{\phi^{*} \partial^{2} \phi}_{-m^{2} \phi^{*} \phi} - (\partial_{\mu} \phi) (\partial^{\mu} \phi^{*}) - \underbrace{\phi \partial^{2} \phi^{*}}_{-m^{2} \phi \phi^{*}} \right]$$
  
$$= 0. \qquad (1.44)$$

The existence and explicit form of the conserved currents will be discussed in connection with Noether's theorem in Section 2.9.

So, the current  $J_{\mu}$  is conserved and can be used to prove time-independence of the norm (as in ordinary quantum mechanics).

#### Current in non-relativistic limit

In non-relativistic limit, we assume that  $\phi(x) = e^{-imt}\varphi(\mathbf{x}, t)$  where  $\varphi(\mathbf{x}, t)$  is supposed to be a non relativistic wave function. By inserting the aforementioned form of  $\phi(x)$  to the explicit form of  $J_{\mu}$  we obtain:

$$J_{NR}(x) = \frac{i}{2m} \left[ \varphi^* \nabla \varphi - (\nabla \varphi)^* \varphi \right],$$
  

$$\rho_{NR}(x) = \frac{i}{2m} \left[ (-im) \varphi \varphi^* + \varphi^* \partial_0 \varphi - (im) \varphi \varphi^* \right]$$
  

$$= \frac{i}{2m} \left[ (-i2m) \varphi \varphi^* \right] = \varphi \varphi *. \qquad (1.45)$$

Here we have neglected the term  $\partial_t \phi$  in comparison to  $-im\phi$ . Eq. (1.45) is the well know form of Schrödinger's conserved probability current and charge (i.e., probability density).

With the conserved current we can now show that the norm is time independent, indeed

$$-\underbrace{\frac{\partial}{\partial t}\int_{V}d^{3}x\rho}_{\text{Change in total probability inside }V} = \int_{V}d^{3}x\nabla \cdot \boldsymbol{J} = \underbrace{\int_{\partial V}d\boldsymbol{S}\cdot\boldsymbol{J}}_{\text{Flux of }\boldsymbol{J}} \to 0. \quad (1.46)$$

Are our integrals convergent?

We want to show that  $\int_{V} d^{3}x \rho$  is finite, so that  $\rho$  could (potentially) represent a density of probability. Since in the non relativistic case  $\rho_N = \phi^* \phi = \varphi \varphi^*$ , we know that the integral (in spherical coordinates)  $\int d\omega dr r^2 |\phi|^2 < \infty$ . Since our fields behave as  $\phi \sim \frac{1}{r^{3/2+\varepsilon}}$ . Our current then has to behave like  $\boldsymbol{J} \sim \phi \boldsymbol{\nabla} \phi \sim \frac{1}{r^{3/2+\varepsilon}} \frac{1}{r^{5/2+\varepsilon}} = \frac{1}{r^{4+\varepsilon}}$ . Since  $\partial V = S^2(R) \sim R^2$  and  $\boldsymbol{J} \sim \frac{1}{R^{4+\varepsilon}}$ , total integral of  $\lim_{R\to\infty} \int_{\partial V} d\boldsymbol{S} \cdot \boldsymbol{J} =$ 0

Let us now show that our norm is relativistically invariant. To this end we can write:

$$||\phi||^{2} = \int d^{3}x \rho(x) = \int d^{4}x \underbrace{\delta(x^{0})}_{\frac{\partial}{\partial x^{0}} \theta(x^{0})} \rho(x)$$
$$= \int d^{4}x J^{\alpha} \frac{\partial}{\partial x^{\alpha}} \theta(n^{\beta}x_{\beta}). \qquad (1.47)$$

Here  $n^{\beta} = (1, 0, 0, 0)$ .

The effect of a Lorentz transformation on  $||\phi||^2$  is then evidently simply to change  $n^{\mu}$ . So, in this connection we define another wave function norm,  $||\widetilde{\phi}||^2$  as

$$||\widetilde{\phi}||^2 = \int \mathrm{d}^4 x J^{\alpha} \frac{\partial}{\partial x^{\alpha}} \theta(n^{\prime\beta} x_{\beta}). \qquad (1.48)$$

Here n' is a generic time-like 4-vector obtained from n via Lorentz transformation, i.e.,  $n'^{\beta} = L^{\beta}_{\gamma} n^{\gamma}$ . Taking difference between two norms we obtain

$$||\phi||^2 - ||\widetilde{\phi}||^2 = \int d^4x J^{\alpha} \frac{\partial}{\partial x^{\alpha}} \left[ \theta(n^{\beta} x_{\beta}) - \theta(n^{\prime \beta} x_{\beta}) \right], \qquad (1.49)$$

Because  $\partial_{\alpha} J^{\alpha} = 0$  (as seen before) we can rewrite expression inside the integral as

$$||\phi||^2 - ||\widetilde{\phi}||^2 = \int d^4x \frac{\partial}{\partial x^{\alpha}} \left[ J^{\alpha} \{ \theta(n^{\beta} x_{\beta}) - \theta(n^{\prime \beta} x_{\beta}) \} \right].$$
(1.50)

By using 4-dimensional version of Gaussian theorem we obtain that

$$||\phi||^2 - ||\widetilde{\phi}||^2 = \int dS_\alpha \left[ J^\alpha \{ \theta(n^\beta x_\beta) - \theta(n^{\prime\beta} x_\beta) \} \right].$$
(1.51)

To show that this is zero, consider two possibilities:

1.  $J^{\alpha}$  can be presumed to vanish if  $|\mathbf{x}| \to \infty$  with fixed *t*.

Time-like vectors have not only dominant time component with respect to space-like components, but in addition, if they are related via Lorentz transform with the vector  $n^{\mu} = (1, 0, 0, 0)$  the have the zero component positive for all orthochronous Lorentz transformations.

2.  $\theta(n^{\beta}x_{\beta}) - \theta(n^{'\beta}x_{\beta})$  vanishes for  $|t| \to \infty$  with *x* fixed.

Hence, the difference is zero and the norm is relativistically invariant (in fact Lorentz scalar) as needed.

Let us now return to the general solution

$$\phi(x) = \int \frac{d^3 p}{(2\pi)^3 2\omega_p} \left[ f(p) e^{-ipx} + g(p) e^{ipx} \right], \quad (1.52)$$

and explore, what its norm would look like:

$$\begin{split} ||\phi||^{2} &= (\phi, \phi) \\ &i \int d^{3}x \left\{ \left[ \int \frac{d^{3}p}{(2\pi)^{3}2\omega_{p}} \left( f^{*}(p)e^{ipx} + g^{*}(p)e^{-ipx} \right) \right. \right. \\ &\times \int \frac{d^{3}q}{(2\pi)^{3}2\omega_{q}} \left( f(q)(-i\omega_{q})e^{-iqx} + g(q)(i\omega_{q})e^{iqx} \right) \right] \\ &- \left[ \int \frac{d^{3}q}{(2\pi)^{3}2\omega_{q}} \left( f(q)e^{-iqx} + g(q)e^{iqx} \right) \right. \\ &\times \int \frac{d^{3}p}{(2\pi)^{3}2\omega_{q}} \left( f^{*}(p)(i\omega_{p})e^{ipx} + g^{*}(p)(-i\omega_{p})e^{-ipx} \right) \right] \right\}.$$
(1.53)

Since our norm is time independent, elements of type  $e^{\pm i(\omega_p + \omega_q)t}$  must cancel, and only terms of the type  $e^{\pm i(\omega_p - \omega_q)t}$  should be considered. Continuing

$$\begin{aligned} ||\phi||^2 &= i \int d^3 \mathbf{x} \int \frac{d^3 \mathbf{p} d^3 \mathbf{q}}{(2\pi)^6 4\omega_p \omega_q} \left[ \left( f^*(\mathbf{p}) f(\mathbf{q}) (-i\omega_q) e^{ix(p-q)} \right) \right. \\ &+ g^*(\mathbf{p}) g(\mathbf{q}) (i\omega_q) e^{-ix(p-q)} \\ &- \left( f(\mathbf{q}) f^*(\mathbf{p}) (i\omega_p) e^{ix(p-q)} \right) \\ &+ g(\mathbf{q}) g^*(\mathbf{p}) (-i\omega_p) e^{-ix(p-q)} \right], \end{aligned}$$
(1.54)

and hence finally we have

$$||\phi||^2 = \int \frac{\mathrm{d}^3 \boldsymbol{p}}{(2\pi)^3 2\omega_p} \left[ |f(\boldsymbol{p})|^2 - |g(\boldsymbol{p})|^2 \right] \,. \tag{1.55}$$

*This norm is not generally positive definite!* However, if we restrict our attention to positive energy only, i.e.,  $g(\mathbf{p}) = 0$ , then  $||\phi||^2$  is positive definite.

#### Note

In a similar spirit as for norm, we can be define the general scalar product between two states as

$$(\psi,\phi) = i \int \mathrm{d}^3 x \left[ \psi^* \partial_0 \phi - \phi (\partial_0 \psi)^* \right].$$

Check that this scalar product is time independent and Lorentz invariant.

We thus see that  $\rho$  cannot represent probability density, it may well be considered (while satisfying continuity equation) as the density of charge (or any other conserved quantity).

Apart from semidefinite probability density, there is a second problem with Klein–Gordon equation. In particular, any plane wave function, i.e.

$$\psi(x) = N e^{\pm i(\omega_p t - \mathbf{p} \cdot \mathbf{x})}, \qquad (1.56)$$

satisfies Klein–Gordon equation, provided that  $E^2 = \omega_p^2 = \mathbf{p}^2 + m^2$ . Thus negative energies  $E = -\sqrt{\mathbf{p}^2 + m^2}$  are on the same footing as the physical ones  $E = \sqrt{\mathbf{p}^2 + m^2}$ . This leads to a problem — energy spectrum is unbounded from below.



**Figure 1.1:** Energy spectrum of a free quantum relativistic particle.

Of course even in classical physics, the relativistic relation  $E^2 = p^2 + m^2$  has two solutions  $E = \pm \sqrt{p^2 + m^2}$ . However, in classical physics we can simply assume that the only physical particles are those with  $E \ge 0$ . This is because the positive-energy solutions have  $E > mc^2$ , while the negative ones have  $E \le -mc^2$ . Hence there is a finite gap between them and in classical (non-quantum) physics there does not exist any continuous process that can take a particle from positive to negative energy.

In relativistic quantum mechanics the problem is more pressing. As Dirac pointed out in 1928 paper [P. A. M. Dirac, Proc. Roy. Soc. A117, 610 (1928)], the interaction of electrons with radiation can produce transition, in which a positive energy electrons falls into a negative energy state, with the energy carried off by two or more photons.



**Figure 1.2:** Spontaneous emission from excited state. For instance, an electron in rest could emit two photon quanta with total energy  $2m_ec^2$  and hence end up in the negative energy level.

This brings about a problem. If we have a quantum particle whose state satisfies the Klein–Gordon equation we could, in principle, extract an arbitrary amount of energy from it (in the form radiated photons). This, in turn, would lead to the perpetuum mobile of the first kind. In addition, when particle reaches the negative energy states there is nothing that would prevent it to decay to even lower energy state. Consequently, the matter (together with us) would be unstable!

# 1.4 Dirac Equation

Klein-Gordon equation is a second order differential equation in time, which can be recognized as a reason why the norm is not positive definite. Dirac sought an equation, that would remedy this "difficulty". It turned out, that by appropriately "linearizing" relativistic wave equation, Dirac arrived (by coincidence) on the wave equation for electron, which indeed provides positive definite probability density. Since the spin is involved, the wave function is not anymore Lorentz scalar (recall Pauli-Schrödinger wave equation, which has as a solution two-component spinor wave function that is not scalar with respect to Galileo group).

Dirac had two goals:

- 1. Equation for wave function that is linear and first order in time derivative. Relativistic invariance then suggests that the equation will also be of first order in spatial derivatives.
- 2. Positive definite norm.

Assume that this equation has the form

$$\left(i\gamma^{0}\frac{\partial}{\partial x^{0}} + i\boldsymbol{\gamma}\cdot\boldsymbol{\nabla}\right)\psi(x) = m\psi(x), \qquad (1.57)$$

which might be written in a shorthand notation

$$(i\gamma_{\mu}\partial^{\mu} - m)\psi(x) = 0. \qquad (1.58)$$

By defining Feynman's slash notation  $\partial = \gamma_{\mu} \partial^{\mu}$  this equation reduces to

$$(i\partial - m)\psi(x) = 0. \tag{1.59}$$

Here  $\{\gamma^{\mu}\} = \{\gamma^{0}, \gamma\}$  are some unspecified numbers or matrices. We require that  $\psi(x)$  should also satisfy Klein-Gordon equation, since Klein–Gordon equation just states that  $p_{\mu}p^{\mu} = m^{2}$ . Multiplying (1.58) by  $(i\gamma_{\nu}\partial^{\nu} + m)$  we get

$$0 = (i\gamma_{\nu}\partial^{\nu} + m)(i\gamma_{\mu}\partial^{\mu} - m)\psi(x) = (-\gamma_{\mu}\gamma_{\nu}\partial^{\mu}\partial^{\nu} - m^{2})\psi(x). \quad (1.60)$$

We can rewrite  $\gamma_{\mu}\gamma_{\nu}\partial^{\mu}\partial^{\nu}$  as

$$\gamma_{\mu}\gamma_{\nu}\partial^{\mu}\partial^{\nu} = \frac{1}{2}\gamma_{\mu}\gamma_{\nu}\partial^{\mu}\partial^{\nu} + \frac{1}{2}\gamma_{\nu}\gamma_{\mu}\partial^{\nu}\partial^{\mu} = \frac{1}{2}\{\gamma_{\mu},\gamma_{\nu}\}\partial^{\mu}\partial^{\nu}, \quad (1.61)$$

where  $\{\gamma_{\mu}, \gamma_{\nu}\} = \gamma_{\mu}\gamma_{\nu} + \gamma_{\nu}\gamma_{\mu}$ . To obtain Klein–Gordon equation we must impose condition

$$\{\gamma_{\mu}, \gamma_{\nu}\} = 2\eta_{\mu\nu}, \quad \{\gamma^{\mu}, \gamma^{\nu}\} = 2\eta^{\mu\nu}.$$
(1.62)

Because  $\gamma^{\mu}\gamma^{\nu}\partial^{\mu}\partial^{\nu} = \partial_{\nu}\partial^{\nu}$  we get  $(\Box + m^2)\psi(x) = 0$ .

#### **Dirac's derivation**

Dirac started with the following ansatz:

$$i\frac{\partial\psi}{\partial t} = \left(\frac{1}{i}\alpha\cdot\nabla + \beta m\right)\psi = H_D\psi, \qquad (1.63)$$

where  $H_D$  is Dirac's Hamiltonian, which should be Hermitian (and hence  $\alpha$  and  $\beta$  are Hermitian). Klein–Gordon equation implies that  $\{\alpha_i, \alpha_k\} = 0, \{\alpha_i, \beta\} = 0$  and  $\alpha_i^2 = \beta^2 = 1$  for  $i \neq k$ . Here  $\{A, B\}$  is a symmetric combination of *A* and *B*. This operation is called *anti-commutator*.

By rewriting Dirac equation (1.58) explicitly as

$$\left(i\gamma^0\partial_0+\gamma^i\partial_i-m\right)\psi = 0, \qquad (1.64)$$

and multiplying it by the inverse of  $\gamma^0$  we get

$$\left[i(\gamma^{0})^{-1}\gamma^{0}\partial_{0} + i(\gamma^{0})^{-1}\gamma^{i}\partial_{i} - (\gamma^{0})^{-1}m\right]\psi = 0, \qquad (1.65)$$

which is equivalent to

$$i\partial_0\psi = \left[\frac{1}{i}(\gamma^0)^{-1}\gamma^i\partial_i + (\gamma^0)^{-1}m\right]\psi.$$
 (1.66)

Consequently we see that  $\alpha = (\gamma^0)^{-1} \gamma$  and  $\beta = (\gamma^0)^{-1}$ . Because  $\{\gamma^0, \gamma^0\} = 2$ , we see that  $\gamma^0 = (\gamma^0)^{-1}$ . From anti-commutation relation for  $\gamma^0$  and  $\gamma^i$  we have that  $\gamma^0 \gamma^i = -\gamma^i \gamma^0$  and from Hermiticity we also have that  $\gamma^0 \gamma^i = (\gamma^0 \gamma^i)^{\dagger} = \gamma^{i\dagger} \gamma^{0\dagger}$ . And from that we see that  $\gamma^0 \gamma^i \gamma^0 = \gamma^{i\dagger} = -\gamma^i (\gamma^0)^2 = -\gamma^i$ .

Relation

$$\{\gamma^{\mu}, \gamma^{\nu}\} = 2\eta^{\mu\nu} \tag{1.67}$$

is known as *Clifford algebra*  $CL_{1,3}(\mathbb{R})$  or simply *Dirac algebra*.

Now we can ask ourselves, what is the smallest dimension of  $\gamma^{\mu}$  in 4-dimensional space. In fact, matrices  $\alpha^{i}$  and  $\beta$  have eigenvalues equal to ±1. For  $i \neq j$  we have

$$det(\alpha^{i}\alpha^{j}) = det(-\alpha^{j}\alpha^{i}) = (-1)^{d} det(\alpha^{j}\alpha^{i}),$$
$$det(\alpha^{i}\beta) = (-1)^{d} det(\beta\alpha^{i}).$$
(1.68)

So, the dimension of  $\alpha^i$ , i = 1, 2, 3 and  $\beta$  must be even. Since for d = 2 there exists only 3 anti-commuting Hermitian matrices — Pauli matrices, we have  $d \ge 4$ . There are many representations of  $CL_{1,3}(\mathbb{R})$  with d > 4 (altought they are rarely used in practice). An explicit representation with d = 4 is provided by matrices

$$\gamma^{0} = \begin{pmatrix} \mathbf{1} & \mathbf{0} \\ \mathbf{0} & -\mathbf{1} \end{pmatrix}, \quad \boldsymbol{\gamma} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ -\boldsymbol{\sigma} & 0 \end{pmatrix}.$$
(1.69)

Here  $\sigma$  are Pauli matrices. This representation is known as *Dirac representation* and is useful when discussing non-relativistic limit of

Pauli matrices by themselves generate Clifford algebra  $CL_{0,3}(\mathbb{R})$  via relation  $\{\sigma_a, \sigma_b\} = 2\delta_{ab}\mathbf{1}$ . This algebra is known as Pauli algebra.

the theory. A useful technical trick, for calculating gamma matrices in Dirac's representation (but also in other representations) is based on properties of tensor product  $\otimes$  on matrices. Because

$$(\boldsymbol{A} \otimes \boldsymbol{B}) \cdot (\boldsymbol{C} \otimes \boldsymbol{D}) = (\boldsymbol{A} \cdot \boldsymbol{C}) \otimes (\boldsymbol{B} \cdot \boldsymbol{D}), \qquad (1.70)$$

and

$$\gamma^0 = \sigma^3 \otimes \mathbb{1}, \quad \gamma = i\sigma^2 \otimes \sigma, \qquad (1.71)$$

and

$$\sigma^i \sigma^j = \delta^{ij} + i \varepsilon^{ijk} \sigma^k \,, \tag{1.72}$$

we can immediately check that  $\gamma$  matrices in Dirac's representation satisfy the defining Dirac algebra (1.67).

## 1.5 Lorentz Invariance of Dirac Equation

Recall that a non-relativistic particle with spin has a wave function  $\psi_{\alpha}(x)$  (Weyl spinor) which transforms under rotation *R* as

$$\psi_{\alpha}(\boldsymbol{x}) \xrightarrow{\boldsymbol{R}} D_{\alpha\beta}(\boldsymbol{R})\psi_{\beta}(\boldsymbol{R}^{-1}\boldsymbol{x}).$$
(1.73)

In a similar way, the Dirac wave function under a Lorentz transformation *L* transforms as

$$\psi(x) \xrightarrow{L} \psi_L(x) = S(L)\psi(L^{-1}x), \qquad (1.74)$$

where S(L) is an appropriate representation of the Lorentz group, that acts in the vector space, in which the Dirac wave function takes its values. From this we see that S(L) should be a  $4 \times 4$  matrix.

In order to show that Dirac's equation is Lorentz invariant we need to show that

$$\left(i\gamma^{\mu}\partial_{\mu}-m\right)\psi_{L}(x) = 0, \qquad (1.75)$$

provided

$$\left(i\gamma^{\mu}\partial_{\mu}-m\right)\psi(x) = 0, \qquad (1.76)$$

is satisfied. To show this we rewrite the left-hand-side (LHS) of (1.75) as

LHS = 
$$(i\gamma^{\mu}\partial_{\mu} - m) S(L)\psi(L^{-1}x)$$
  
=  $S(L) [iS^{-1}(L)\gamma^{\mu}\partial_{\mu}S(L) - m] \psi(L^{-1}x)$   
=  $S(L) [iS^{-1}(L)\gamma^{\mu}\partial_{\mu}S(L) - m] \psi(x'),$  (1.77)

where  $x' = L^{-1}x$ . If we can find an appropriate matrix *S*(*L*) such that

$$S^{-1}(L)\gamma^{\mu}\partial_{\mu}S(L) = \gamma^{\mu}\partial'_{\mu}, \qquad (1.78)$$

then

$$(i\gamma^{\mu}\partial_{\mu} - m)\psi_{L}(x) = S(L)(i\gamma^{\mu}\partial_{\mu}' - m)\psi(x').$$
(1.79)

Since  $\psi$  is a Dirac wave function, then

$$\left(i\gamma^{\mu}\partial'_{\mu}-m\right)\psi(x') = 0 \quad \Rightarrow \quad \left(i\gamma^{\mu}\partial_{\mu}-m\right)\psi_{L}(x) = 0. \tag{1.80}$$

Consequently, also  $\psi_L$  is Dirac's wave function and Dirac's equation is relativistically invariant provided such S(L) exists. To find S(L) we have to explore properties of Lorentz group in more detail.

#### Lorentz group

From the condition (1.6) we know that there exist 2 kinds of Lorentz transformations — proper (those with det L = 1) and improper (those with det L = -1). We can expand this classification even further by realizing that

$$1 = \eta^{00} = L^{0}_{\nu} L^{0}_{\nu'} \eta^{\nu\nu'} = (L^{0}_{0})^{2} - \sum_{i=1}^{3} (L^{0}_{i})^{2}.$$
(1.81)

Rewriting this we arrive at the condition

$$(L_0^0)^2 = 1 + \sum_{i=1}^3 (L_i^0)^2.$$
 (1.82)

Lorentz transformations for which  $L_0^0 \ge 1$  are called *orthochronous* transformations, those with  $L_0^0 \le -1$  are called *non-orthochronous*. We can not switch between those four types of Lorentz transformations using continuous process. Transitions between these disconnected parts of the Lorentz group can be done only via discrete transformations such as *parity* or *time reversal* (see Chapter 1.11).

Let us recall (Chapter 2.2.) that Lorentz group has 6 independent parameters  $\omega_{\mu\nu} = -\omega_{\nu\mu}$  that define it. In terms of these we can construct finite Lorentz transformations as

$$L^{\rho}_{\ \tau} = \left(e^{-\frac{i}{4}M^{\mu\nu}\omega_{\mu\nu}}\right)^{\rho}_{\ \tau}.$$
 (1.83)

Here  $M^{\mu\nu}$  are so-called generators of Lorentz transformation, which are fixed by comparison with the infinitesimal transformation (i.e., when when  $\|\omega_{\mu\nu}\| \ll 1$ ). In Chapter 1.2 we have found that

$$(M^{\mu\nu})^{\rho}{}_{\tau} = 2i \left( g^{\rho\mu} \delta^{\nu}_{\tau} - g^{\rho\nu} \delta^{\mu}_{\tau} \right) . \tag{1.84}$$

#### **Rotation group**

To proceed, we start with a familiar example — *rotation group*. Elements of a rotation group are defined by

$$\boldsymbol{R}_{ij} = \left(e^{-i\theta\boldsymbol{n}_k\boldsymbol{J}_k}\right)_{ij} = \left(e^{-i\omega_k\boldsymbol{J}_k}\right)_{ij}, \qquad (1.85)$$

Since now  $x'^{\mu} = (L^{-1})^{\mu}_{\nu} x^{\nu}$  we have that  $x^{\mu} = L^{\mu}_{\nu} x'^{\nu}$  and thus  $\partial'_{\mu} = \frac{\partial x^{\nu}}{\partial x'^{\mu}} \frac{\partial}{\partial x^{\nu}} = L^{\nu}_{\mu} \frac{\partial}{\partial x^{\nu}}$ .

where *n* is a unit vector along the axis of rotation. Group generators  $J_i$  satisfy the usual angular momentum commutation relations

$$\left[\boldsymbol{J}_{i}, \boldsymbol{J}_{j}\right] = i\varepsilon_{ijk}\boldsymbol{J}_{k}. \qquad (1.86)$$

Recall from quantum mechanics that *vector operators* are sets of 3 operators, say  $V_i(\mathbf{x})$  that transform according to

$$U(\boldsymbol{R})^{\dagger} V_{i}(\boldsymbol{x}) U(\boldsymbol{R}) = \sum_{j} \boldsymbol{R}_{ij} V_{j}(\boldsymbol{x}). \qquad (1.87)$$

For infinitesimal rotations one obtains

$$(1 + i\omega_k \mathbb{J}_k) V_i (1 - i\omega_k \mathbb{J}_k) = [1 - i\omega_k (J_k)_{ij}] V_j.$$
(1.88)

Here  $\mathbb{J}_k$  are operators of angular momentum, acting on corresponding state space (e.g.  $L^2(\mathbb{R})$ ) and  $(J_k)_{ij}$  is a vector representation of angular momentum in 3D, which is known to be

$$\boldsymbol{J}_{1} = i \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -1 \\ 0 & 1 & 0 \end{pmatrix}, \quad \boldsymbol{J}_{2} = i \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \\ -1 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{J}_{3} = i \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (1.89)$$

This can succinctly be written as:  $(J_j)_{ik} = i\varepsilon_{ijk}$ .

After algebraic manipulations we obtain from (1.88)

$$i\omega_k\left[\mathbb{J}_k, V_i\right] = -i\omega_k(\mathbf{J}_k)_{ij}V_j, \qquad (1.90)$$

which then implies that

$$[\mathbb{J}_k, V_i] = -(\mathbf{J}_k)_{ij} V_j = -i\varepsilon_{ikj} V_j = i\varepsilon_{kij} V_j.$$
(1.91)

This relation represents an algebraic condition for vector operators. As a byproduct we see that the generators  $J_k$  themselves are vector operators.

#### Adjoint representation

Representations where elements (group generators)  $A_i$  of algebra  $[A_i, A_j] = c_{ikj}A_k$  are defined via structure constants  $c_{ikj}$  so that  $(A_i)_{jk} = c_{ikj}$  are called *adjoint* or *regular* representations.

#### Lorentz group

From the representation of the generators (1.84) we can deduce the commutation relations determining the Lie algebra of Lorentz group. In particular, we find that

$$\left[\boldsymbol{M}^{\mu\nu}, \boldsymbol{M}^{\alpha\beta}\right] = 2i \left\{ \boldsymbol{g}^{\mu\beta} \boldsymbol{M}^{\nu\alpha} + \boldsymbol{g}^{\nu\alpha} \boldsymbol{M}^{\mu\beta} - \boldsymbol{g}^{\mu\alpha} \boldsymbol{M}^{\nu\beta} - \boldsymbol{g}^{\nu\beta} \boldsymbol{M}^{\mu\alpha} \right\}.$$
(1.92)

Here  $U(\mathbf{R})$  is a representation of rotation group which acts on state space (e.g.  $L^2(\mathbb{R})$ ) and  $\mathbf{R}_{ij}$  is a representation of rotation group that acts on the operator indices.

For *M*<sup>*ij*</sup>, *i*, *j* = 1, 2, 3 we have

$$\begin{bmatrix} M^{12}, M^{13} \end{bmatrix} = 2iM^{23},$$
$$\begin{bmatrix} M^{23}, M^{12} \end{bmatrix} = -2iM^{31},$$
(1.93)

etc. Defining

$$\boldsymbol{J}_{i} = \frac{1}{4} \varepsilon_{ijk} \boldsymbol{M}^{jk} \iff \boldsymbol{M}^{jk} = 2\varepsilon^{jki} \boldsymbol{J}_{i}, \qquad (1.94)$$

then from (1.93) we have

$$[\mathbf{J}_{3}, (-\mathbf{J}_{2})] = i\mathbf{J}_{1} \iff [\mathbf{J}_{2}, \mathbf{J}_{3}] = i\mathbf{J}_{1},$$
$$[\mathbf{J}_{1}, \mathbf{J}_{3}] = -i\mathbf{J}_{2}. \tag{1.95}$$

It can be easily checked that we can generally write

$$[\boldsymbol{J}_i, \boldsymbol{J}_j] = i\varepsilon_{ijk}\boldsymbol{J}_k. \tag{1.96}$$

From this we see that  $J_i$  are generators of rotations, since they close the familiar Lie algebra for group of rotations in 3-dimensional space, i.e.,  $SO(3) \sim SU(2)$ .

Similarly we can define

$$M^{0i} = 2K^i . (1.97)$$

From this we see, for instance, that

$$[\mathbf{M}^{01}, \mathbf{M}^{02}] = -2i\mathbf{M}^{12} \implies [\mathbf{K}^1, \mathbf{K}^2] = -i\mathbf{J}^3.$$
(1.98)

It can again be checked that one generally has

$$[\mathbf{K}^{i}, \mathbf{K}^{j}] = -i\varepsilon^{ijk} \mathbf{J}_{k} \iff [\mathbf{K}_{i}, \mathbf{K}_{j}] = -i\varepsilon_{ijk} \mathbf{J}_{k}.$$
(1.99)

Here  $K_i$  are the so-called *generators of boosts* in *i*-th direction. A precise meaning of this terminology will be clarified in Chapter 1.7.

To close the algebra we also need commutators of the type [J, K]. It can be verified that

$$[\boldsymbol{J}_i, \boldsymbol{K}_j] = i\varepsilon_{ijk}\boldsymbol{K}_k. \qquad (1.100)$$

So, the Lie algebra (1.92) can be equivalently rewritten as

$$[\boldsymbol{J}_i, \boldsymbol{J}_j] = i\varepsilon_{ijk}\boldsymbol{J}_k,$$
  
$$[\boldsymbol{J}_i, \boldsymbol{K}_j] = i\varepsilon_{ijk}\boldsymbol{K}_k,$$
  
$$[\boldsymbol{K}_i, \boldsymbol{K}_j] = -i\varepsilon_{ijk}\boldsymbol{J}_k.$$
 (1.101)

These commutation relations define SO(3, 1) algebra. Note that the first commutation relation implies that algebra SO(3) is a subalgebra of SO(3, 1) algebra. On the other hand, boosts do not form a subalgebra of SO(3, 1), so we need both boosts and rotations to form closed algebra.

Group of Lorentz transformations — terminology

*Defining* or *fundamental* representation of *SO*(3, 1) group is given by matrices satisfying the defining relation

$$x^{\mathsf{T}}x = (\mathbf{L}x)^{\mathsf{T}}(\mathbf{L}x) = x^{\mathsf{T}}\mathbf{L}^{\mathsf{T}}\mathbf{L}x = \text{invariant}.$$

From this we can explicitly write that  $L^{\mathsf{T}}L = \mathbf{1}$  (i.e.,  $L_{\mu}{}^{\nu}L^{\mu}{}_{\alpha} = \delta^{\nu}{}_{\alpha}$ ) and hence  $L^{\mathsf{T}} = L^{-1}$ . From this we can see that L are orthogonal matrices preserving the spacetime distance  $x_0^2 - \sum_{i=1}^3 x_i^2$ . Those matrices are of O(3, 1) type and since det L = 1 for proper transformations, we stress this extra fact in "*S*" in the *SO*(3, 1) group name.

Commutation relations can be diagonalized via transformation

$$N_i = \frac{1}{2}(J_i + iK_i), \quad N_i^{\dagger} = \frac{1}{2}(J_i - iK_i). \quad (1.102)$$

From this follows that

$$[N_i, N_j^{\dagger}] = 0, \ [N_i, N_j] = i\varepsilon_{ijk}N_k, \ [N_i^{\dagger}, N_j^{\dagger}] = i\varepsilon_{ijk}N_k^{\dagger}.$$
 (1.103)

The relation  $[N_i, N_j] = i\varepsilon_{ijk}N_k$  (and the same for  $N^{\dagger}$ ) close the SU(2) algebra. Hence, we can view SO(3, 1) algebra as being isomorphic to  $SU(2) \oplus SU(2) \sim SL(2, \mathbb{C})$ . For SU(2) algebra we can define *Casimir* operator. For  $N_i$  and  $N_i^{\dagger}$ ) the latter can be defined as  $\sum_{i=1}^3 N_i^2 = n(n+1)$  and  $\sum_{i=1}^3 N_i^{\dagger 2} = m(m+1)$ . Constants n and m describe nothing but the size of the angular momenta (or spin). The representation of SO(3, 1) can then be denoted with the pair (n, m). Note, in particular, that the transformation with respect to spatial parity is given by

$$\underbrace{\boldsymbol{J}_i \xrightarrow{\boldsymbol{P}} \boldsymbol{J}_i}_{\text{seudovector}} \quad \text{and} \quad \underbrace{\boldsymbol{K}_i \xrightarrow{\boldsymbol{P}} - \boldsymbol{K}_i}_{\text{Vector}}, \quad (1.104)$$

and hence

$$N_i \stackrel{P}{\leftrightarrow} N_i^{\dagger} \Rightarrow (n,m) \stackrel{P}{\leftrightarrow} (m,n).$$
 (1.105)

Generally representations of Lorentz group need not to be parity invariant (for example parity is violated in weak interactions). In addition, since  $J_i = N_i + N_i^{\dagger}$ , we can identify the spin of representation (n + m), e.g., spin-0 particle is described (i.e, its wave function is) in the representation (0, 0), spin-1/2 particle can be in (parity non-invariant) representations (1/2, 0) or (0, 1/2) while spin-1 particle can be in representations (1/2, 1/2) or (1, 0) or (0, 1).

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#### Spin 1/2 representations

Representation (1/2, 0) is known as a *left-handed spinor* (handedness is a convention), while the representation (0, 1/2) is known as a *right-handed spinor*. Corresponding wave functions are typically

This diagonalization does not provide Hermitian generators!

Parity violation was experimentally observed in week interactions (namely in the pion decay) in 1956 by the Chinese American physicist Chien-Shiung Wu. 2-component objects that are called Weyl spinors.

When parity is relevant, one considers the linear combination  $(0, 1/2) \oplus (1/2, 0)$ , which yields 4-component wave function known as a *Dirac spinor* or *bispinor*.

#### Lorentz Invariance of Dirac Equation Continued

Our goal is to show that the Dirac equation transforms covariantly under Lorentz transformations. So, we equivalently, we require that the Lorentz transformed wave function

$$\psi(x) \xrightarrow{L} \psi_L(x) = S(L)\psi(L^{-1}x), \qquad (1.106)$$

should satisfy Dirac's equation provided  $\psi(\mathbf{x})$  does. Here  $S(\mathbf{L})$  is a representation of the Lorentz group that acts only on the indices of wave function  $\psi$ . As such, it must satisfy the group composition law  $S(\mathbf{L}_1)S(\mathbf{L}_2) = S(\mathbf{L}_1\mathbf{L}_2)$ . On the other hand, Dirac's equation transforms covariantly provided that

$$S^{-1}(L)\gamma^{\mu}S(L) = L^{\mu}{}_{\nu}\gamma^{\nu}. \qquad (1.107)$$

It can be easily checked that this condition is compatible with the group composition law and so S(L) is a representation of the Lorentz group. Question now stand how look the corresponding generators and to what representation they belong to. This information can be obtained by considering an infinitisemal Lorentz transformation. In particular, in such a case we can write

$$L = 1 - \frac{i}{4} M^{\mu\nu} \omega_{\mu\nu}, \qquad (1.108)$$

and correspondingly

$$S(L) = 1 - \frac{i}{4} \sigma^{\mu\nu} \omega_{\mu\nu}. \qquad (1.109)$$

Here  $\sigma^{\mu\nu}$  are the generators of the Lorentz group in the representation that is appropriate to Dirac space (space of Dirac's wave functions — bispinors). Analogously

$$S^{-1}(L) = S(L^{-1}) = \mathbb{1} + \frac{i}{4}\sigma^{\mu\nu}\omega_{\mu\nu}. \qquad (1.110)$$

Inserting this into (1.107) we obtain that

$$\left(\mathbb{1} + \frac{i}{4}\sigma^{\mu\nu}\omega_{\mu\nu}\right)\gamma^{\rho}\left(\mathbb{1} - \frac{i}{4}\sigma^{\mu\nu}\omega_{\mu\nu}\right) = \left(\delta^{\rho}_{\tau} + \omega^{\rho}_{\tau}\right)\gamma^{\tau}, \qquad (1.111)$$

and thus

$$\frac{i}{4} [\sigma^{\mu\nu} \omega_{\mu\nu}, \gamma^{\rho}] = \omega^{\rho}_{\tau} \gamma^{\tau} . \qquad (1.112)$$

By writing

$$\omega^{\rho}{}_{\tau}\gamma^{\tau} = \omega_{\mu\nu}\eta^{\mu\rho}\gamma^{\nu} = \frac{1}{2}\omega_{\mu\nu}(\eta^{\mu\rho}\gamma^{\nu} - \eta^{\nu\rho}\gamma^{\mu}). \qquad (1.113)$$

So, in particular  $S(L)S(L^{-1}) = S(1) = 1$ and hence  $S(L^{-1}) = S^{-1}(L)$ .

Again we are dealing with connected part of the Lorentz group that contains the unit element. Eq. (1.112) can be rewritten as

This should determine the Dirac representation generators  $\sigma^{\mu\nu}$ .

$$\frac{i}{4}[\sigma^{\mu\nu},\gamma^{\rho}] = \frac{1}{2}(\eta^{\mu\rho}\gamma^{\nu} - \eta^{\nu\rho}\gamma^{\mu}). \qquad (1.114)$$

This condition is satisfied if  $\sigma^{\mu\nu} = \frac{i}{2} [\gamma^{\mu}, \gamma^{\nu}]$ . Indeed, by using the well known identity  $[AB, C] = A\{B, C\} - \{A, C\}B$  we can write

$$\frac{i}{4} \left( \frac{i}{2} [\gamma^{\mu} \gamma^{\nu}, \gamma^{\rho}] - \frac{i}{2} [\gamma^{\nu} \gamma^{\mu}, \gamma^{\rho}] \right)$$

$$= -\frac{1}{8} (\gamma^{\mu} \{\gamma^{\nu}, \gamma^{\rho}\} - \{\gamma^{\mu}, \gamma^{\rho}\} \gamma^{\nu} - \gamma^{\nu} \{\gamma^{\mu}, \gamma^{\rho}\} + \{\gamma^{\nu}, \gamma^{\rho}\} \gamma^{\mu})$$

$$= -\frac{1}{8} (2\gamma^{\mu} \eta^{\nu\rho} - 2\eta^{\mu\rho} \gamma^{\nu} - 2\gamma^{\nu} \eta^{\mu\rho} + 2\eta^{\nu\rho} \gamma^{\mu})$$

$$= \frac{1}{2} (\gamma^{\nu} \eta^{\mu\rho} - \gamma^{\mu} \eta^{\nu\rho}) .$$
(1.115)

It can also be checked that generators  $\sigma^{\mu\nu} = \frac{i}{2}[\gamma^{\mu}, \gamma^{\nu}]$  satisfy the correct Lorentz group algebra

$$[\sigma^{\mu\nu},\sigma^{\alpha\beta}] = 2i \left\{ \eta^{\mu\beta}\sigma^{\nu\alpha} + \eta^{\nu\alpha}\sigma^{\mu\beta} - \eta^{\mu\alpha}\sigma^{\nu\beta} - \eta^{\nu\beta}\sigma^{\mu\alpha} \right\}.$$
(1.116)

Finally we can write that the finite Lorentz transformations S(L) have the form

$$S(L) = e^{-\frac{i}{4}\sigma^{\mu\nu}\omega_{\mu\nu}}$$
 with  $L = e^{-\frac{i}{4}M^{\mu\nu}\omega_{\mu\nu}}$ . (1.117)

This closes our proof of the Lorentz covariance of the Dirac equation.

# **1.6 Dirac Bilinears**

Dirac bilinears are relevant for construction of observables in quantum field theory but they will also help us to construct other quantities of interest, e.g., probability current.

First, general Dirac's wave function has form

$$\psi(x) = \begin{pmatrix} \psi_1(x) \\ \psi_2(x) \\ \psi_3(x) \\ \psi_4(x) \end{pmatrix}, \quad \psi^{\dagger}(x) = (\psi_1^*(x), \psi_2^*(x), \psi_3^*(x), \psi_4^*(x)). \quad (1.118)$$

We define *spinor adjoint* to  $\psi$  as

$$\overline{\psi}(x) = \psi^{\dagger}(x)\gamma^{0}. \qquad (1.119)$$

Let us first see how  $\overline{\psi}(x)$  transforms under the Lorentz transformation. To this end we use two simple facts, namely

$$\begin{split} \psi(x) &\xrightarrow{L} \psi_{L}(x) = S(L)\psi(L^{-1}x) \\ \psi^{\dagger}(x) &\xrightarrow{L} \psi_{L}^{\dagger}(x) = \psi^{\dagger}(L^{-1}x)S^{\dagger}(L) \,. \end{split}$$
(1.120)

Now, we can multiply from right the second equation by  $\gamma^0$ , i.e.

$$\overline{\psi}(x) = \psi^{\dagger}(x)\gamma^{0} \xrightarrow{L} \psi^{\dagger}_{L}(x)\gamma^{0} = \psi^{\dagger}(L^{-1}x)S^{\dagger}(L)\gamma^{0}.$$
(1.121)

We now use the fact that

$$S(L) = e^{-\frac{i}{4}\sigma^{\mu\nu}\omega_{\mu\nu}} \implies S^{\dagger}(L) = e^{\frac{i}{4}(\sigma^{\mu\nu})^{\dagger}\omega_{\mu\nu}}, \qquad (1.122)$$

where  $(\sigma^{\mu\nu})^{\dagger}$  is

$$(\boldsymbol{\sigma}^{\mu\nu})^{\dagger} = \left(\frac{i}{2}[\gamma^{\mu},\gamma^{\nu}]\right)^{\dagger} = -\frac{i}{2}[\gamma^{\nu\dagger},\gamma^{\mu\dagger}] = \frac{i}{2}[\gamma^{\mu\dagger},\gamma^{\nu\dagger}]. \quad (1.123)$$

How do we "rotate"  $\gamma^{\nu \dagger}$  to  $\gamma^{\nu ?}$  By writing Dirac equation in Schrödinger like form, i.e.

$$i\partial_t \psi = -i\gamma^0 \gamma^i \partial_i \psi + \gamma^0 m \psi \equiv \boldsymbol{H}_D \psi , \qquad (1.124)$$

 $(H_D$  is a Dirac Hamiltonian) we get from the presumed hermiticity of  $H_D$  that

$$\begin{aligned} \gamma^{0} &= \gamma^{0\dagger} \\ \gamma^{i\dagger} &= -\gamma^{i} = -\gamma^{0}\gamma^{0}\gamma^{0}\gamma^{i} = \gamma^{0}\gamma^{i}\gamma^{0}. \end{aligned} \tag{1.125}$$

Those identities are valid irrespective of chosen representation and a particular example of  $\gamma$ -matrices that satisfy these conditions is provided by the oldest representation of Dirac matrices that is due to Dirac himself, i.e.

$$\begin{split} \gamma^{0} &= \sigma^{3} \otimes \mathbb{1} = \begin{pmatrix} \mathbb{1} & 0\\ 0 & -\mathbb{1} \end{pmatrix}, \\ \gamma^{i} &= i\sigma^{2} \otimes \sigma^{i} = \begin{pmatrix} 0 & \sigma^{i}\\ -\sigma^{i} & 0 \end{pmatrix}. \end{split}$$
(1.126)

#### Some properties of $\gamma$ -matrices

Here we summaries some important properties of  $\gamma$ -matrices.

• 
$$\gamma^0 = (\gamma^0)^{-1}, (\gamma^0)^2 = 1$$
 and  $(\gamma^0)^{\dagger} = \gamma^0$ 

$$\blacktriangleright$$
  $(\gamma^i)^{\dagger} = -\gamma^i$ 

$$\blacktriangleright \gamma^0(\gamma^0)^{\dagger}\gamma^0 = \gamma^0\gamma^0\gamma^0 = \gamma^0$$

 $\blacktriangleright \gamma^0(\gamma^i)^{\dagger}\gamma^0 = -\gamma^0\gamma^i\gamma^0 = \gamma^i$ 

$$\blacktriangleright \gamma^0 (\gamma^\mu)^\dagger \gamma^0 = \gamma^\mu$$

 $\blacktriangleright \gamma^0(\sigma^{\mu\nu})^{\dagger}\gamma^0 = \gamma^0 \frac{1}{2} [(\gamma^{\mu})^{\dagger}, (\gamma^{\nu})^{\dagger}]\gamma^0 = \frac{i}{2} (\gamma^{\mu}\gamma^{\nu} - \gamma^{\nu}\gamma^{\mu}) = \sigma^{\mu\nu}$ 

Now consider

$$\gamma^{0}S(L)^{\dagger}\gamma^{0} = e^{\frac{i}{4}\omega_{\mu\nu}\gamma^{0}(\sigma^{\mu\nu})^{\dagger}\gamma^{0}} = e^{\frac{i}{4}\omega_{\mu\nu}\sigma^{\mu\nu}} = (S(L))^{-1}.$$
(1.127)

So  $\gamma^0 S(L)^{\dagger} \gamma^0 = S^{-1}(L) = S(L^{-1})$ . From this it follows that

$$\overline{\psi}(x) = \psi^{\dagger}(x)\gamma^{0} \xrightarrow{L} \psi^{\dagger}(L^{-1}x)S^{\dagger}(L)\gamma^{0}$$
$$= \psi^{\dagger}(L^{-1}x)\gamma^{0}\gamma^{0}S(L)^{\dagger}\gamma^{0}$$
$$= \overline{\psi}(L^{-1}x)S^{-1}(L). \qquad (1.128)$$

So finally we have the following transformation rules

$$\psi(x) \xrightarrow{L} \psi_L(x) = S(L)\psi(L^{-1}x),$$
  
$$\overline{\psi}(x) \xrightarrow{L} \overline{\psi}_L(x) = \overline{\psi}(L^{-1}x)S^{-1}(L).$$
(1.129)

These relations are key in forming bilinears.

#### **Classification of bilinears**

First, we begin with scalar bilinears

$$\overline{\psi}(x)\psi(x) \xrightarrow{L} \overline{\psi}_{L}(x)\psi_{L}(x) = \overline{\psi}(L^{-1}x)S^{-1}(L)S(L)\psi(L^{-1}x)$$
$$= \overline{\psi}(L^{-1}x)\psi(L^{-1}x) \equiv s(x). \quad (1.130)$$

Which can be rewritten as

$$s(x) \xrightarrow{L} s_L(x) = s(L^{-1}x).$$
(1.131)

This is transformation property of scalar field. Next, the *vector fields* (or vector currents) are defined as

$$J^{\mu}(x) = \overline{\psi}(x)\gamma^{\mu}\psi(x). \qquad (1.132)$$

Transforming this current we obtain

$$J^{\mu}(x) \xrightarrow{L} J^{\mu}_{L}(x) = \overline{\psi}_{L}(x)\gamma^{\mu}\psi_{L}(x)$$
$$= \overline{\psi}(L^{-1}x)S^{-1}(L)\gamma^{\mu}S(L)\psi(L^{-1}x). \quad (1.133)$$

By recalling that the following relation for  $\gamma$ -matrices holds

$$S^{-1}(L)\gamma^{\mu}S(L) = L^{\mu}{}_{\nu}\gamma^{\nu}, \qquad (1.134)$$

we get

$$J_{\boldsymbol{L}}^{\mu}(x) = \overline{\psi}(\boldsymbol{L}^{-1}x)\boldsymbol{L}^{\mu}{}_{\nu}\gamma^{\nu}\psi(\boldsymbol{L}^{-1}x)$$
$$= \boldsymbol{L}^{\mu}{}_{\nu}\overline{\psi}(\boldsymbol{L}^{-1}x)\gamma^{\nu}\psi(\boldsymbol{L}^{-1}x). \qquad (1.135)$$

Thus

$$J_{L}^{\mu}(x) = L^{\mu}{}_{\nu}\overline{\psi}(L^{-1}x)\gamma^{\nu}\psi(L^{-1}x) = L^{\mu}{}_{\nu}J^{\nu}(L^{-1}x).$$
(1.136)

This is indeed the correct transformation law for a vector field.

In order to discuss *pseudoscalars* and *pseudovectors*, we will introduce a new  $\gamma$ -matrix, namely

$$\gamma^5 = i\gamma^0 \gamma^1 \gamma^2 \gamma^3 \,, \tag{1.137}$$

which in the Dirac representation has the form

$$\gamma^5 = \sigma^1 \otimes \mathbb{1} = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}.$$
(1.138)

**Basic properties of**  $\gamma^5$ 

•  $(\gamma^5)^{\dagger} = \gamma^5$ •  $(\gamma^5)^2 = 1$ •  $\{\gamma^5, \gamma^{\mu}\} = 0 \text{ for } \mu = 0, 1, 2, 3$ 

Now, the bilinear

$$P(x) = \overline{\psi}(x)\gamma^5\psi(x) \tag{1.139}$$

is a *pseudoscalar*, i.e. under standard (proper) Lorentz transformation it behaves like a scalar but changes its sign under the parity transformation. To see this, let us realize that

$$\gamma^5 = -i\gamma^1\gamma^0\gamma^2\gamma^3 = i\gamma^1\gamma^0\gamma^3\gamma^2 = \frac{i}{4!}\varepsilon_{\mu\nu\sigma\tau}\gamma^\mu\gamma^\nu\gamma^\sigma\gamma^\tau, \quad (1.140)$$

and also that (all involved indices are distinct)

$$\varepsilon^{\mu\nu\sigma\tau}\gamma^5 = i\gamma^{\mu}\gamma^{\nu}\gamma^{\sigma}\gamma^{\tau}. \qquad (1.141)$$

Here  $\varepsilon_{\mu\nu\sigma\tau}$  is a permutation symbol (4D analogue of Levi–Civita symbol):

$$\varepsilon_{\mu\nu\sigma\tau} = 1$$
 if  $(\mu\nu\sigma\tau)$  is even permutation of (0123),  
 $\varepsilon_{\mu\nu\sigma\tau} = -1$  if  $(\mu\nu\sigma\tau)$  is odd permutation of (0123),  
 $\varepsilon_{\mu\nu\sigma\tau} = 0$  therwise. (1.142)

Continuing from (1.139) we have

$$P(x) = \overline{\psi}(x)\gamma^{5}\psi(x) \xrightarrow{L} \overline{\psi}_{L}(x)\gamma^{5}\psi_{L}(x)$$
$$= \overline{\psi}(L^{-1}x)S^{-1}(L)\gamma^{5}S(L)\psi(L^{-1}x). \quad (1.143)$$

We can rewrite term  $S^{-1}(L)\gamma^5 S(L)$  as follows:

$$S^{-1}(L)\gamma^{5}S(L) = \frac{i}{4!}\varepsilon_{\mu\nu\sigma\tau}S^{-1}(L)\gamma^{\mu}\gamma^{\nu}\gamma^{\sigma}\gamma^{\tau}S(L)$$

$$= \frac{i}{4}\varepsilon_{\mu\nu\sigma\tau}(S^{-1}(L)\gamma^{\mu}S(L))\dots(S^{-1}(L)\gamma^{\tau}S(L))$$

$$= \frac{i}{4!}\varepsilon_{\mu\nu\sigma\tau}L^{\mu}{}_{\mu'}L^{\nu}{}_{\nu'}L^{\sigma}{}_{\sigma'}L^{\tau}{}_{\tau'}\gamma^{\mu'}\gamma^{\nu'}\gamma^{\sigma'}\gamma^{\tau'}$$

$$= \gamma^{5}(\det L). \qquad (1.144)$$

Here we have used the fact that

$$\det A = \sum_{\{J_i\}} \varepsilon_{J_1,\dots,J_n} A_{1J_1}\dots A_{nJ_n}$$
$$= \frac{1}{n!} \sum_{\{J_i\}} \sum_{\{k_i\}} \varepsilon_{J_1,\dots,J_n} \varepsilon_{K_1,\dots,K_n} A_{K_1,J_1}\dots A_{K_n,J_n} . \quad (1.145)$$

Consequently

$$P(x) = \overline{\psi}(x)\gamma^5\psi(x) \xrightarrow{L} \det L\overline{\psi}_L(x)\gamma^5\psi_L(x) = \det LP(L^{-1}x),$$

and the function P(x) is a Lorentz scalar for all proper Lorentz transformations (det L = 1).

Notice that for the Lorentz transformations involving parity reversal

$$L^{P} = \operatorname{diag}(1, -1, -1, -1), \qquad (1.146)$$

the transformation also changes sign as det  $L^P = -1$ . Complete set of bilinears is given in the following table. Note that all bilinears present in Tab. 1.1 have the form  $\overline{\psi}(x)\Gamma_i\psi(x)$ , where  $\Gamma_i$  is one of 16 possible

Table 1.1: List of Dirac's bilinears.

Bilinear	Transformation properties
$\overline{\psi}(x)\psi(x)$	Scalar
$\overline{\psi}(x)\gamma^5\psi(x)$	Pseudoscalar
$\overline{\psi}(x)\gamma^{\mu}\gamma^{5}\psi(x)$	Pseudovector field
$\overline{\psi}(x)\gamma^{\mu}\psi(x)$	Vector field
$\overline{\psi}(x)[\gamma^{\mu},\gamma^{\nu}]\psi(x)$	Antisymmetric tensor field

matrices: 1,  $\gamma^{\mu}$ ,  $[\gamma^{\mu}, \gamma^{\nu}]$ ,  $\gamma^{5}$  and  $\gamma^{5}\gamma^{\mu}$ . There is no way how to build *symmetric* tensor out of bilinears.

Basic properties of $\Gamma_i$ matrices		
► apart from $\Gamma_1 = \mathbb{1}$ we have that $\text{Tr}(\Gamma_i) = 0$		
▶ apart from $\Gamma_1 = \mathbb{1}$ we have that $\Gamma_i \Gamma_j = -\Gamma_j \Gamma_i$		
$\blacktriangleright \Gamma_i^2 = \pm \mathbb{1}$		
► $\operatorname{Tr}(\Gamma_i \Gamma_j) = 0$ for $i \neq j$ and $\operatorname{Tr}(\Gamma_i^2) = \pm 4$		
$\blacktriangleright \sum_{i=1}^{16} \alpha_i \Gamma_i = 0 \text{ iff all } \alpha_i = 0$		
So, $\Gamma_i$ matrices form a basis in the space of $4 \times 4$ matrices.		

# 1.7 Current for a Dirac wave function

Main motivation of Dirac was to have consistent probability current with positive definite probability density. There is now a natural candidate for a probability current, namely

$$J_{\mu}(x) = \overline{\psi}(x)\gamma_{\mu}\psi(x). \qquad (1.147)$$

By analogy with non-relativistic quantum mechanics one can define the norm via current as

$$(\psi,\psi) = ||\psi||^2 = \int d^3x J_0(x) = \int dV n^{\mu} J_{\mu}(x).$$
 (1.148)

The last integral is over a space-like hyperplane orthogonal to the (time-like) 4-vector  $n^{\mu}$ . We want to show the following:

- ►  $||\psi||^2$  is time independent.
- ►  $||\psi||^2$  is a Lorentz invariant norm.

In order to prove time independence of  $||\psi||^2$  we show first that  $\partial_{\mu}J^{\mu}(x) = 0$ . To this end we need to compute

$$\partial_{\mu}\left(\overline{\psi}(x)\gamma^{\mu}\psi(x)\right) = \left(\partial_{\mu}\overline{\psi}(x)\right)\gamma^{\mu}\psi(x) + \overline{\psi}(x)\gamma^{\mu}\left(\partial_{\mu}\psi(x)\right). \quad (1.149)$$

Recalling that  $(i\gamma^{\mu}\partial_{\mu} - m)\psi(x) = 0$  we have

$$\gamma^{\mu}\partial_{\mu}\psi(x) = -im\psi(x). \qquad (1.150)$$

For the adjoint wave function  $\overline{\psi}$  we obtain an equation of motion by taking first the hermitian conjugation of Dirac's equation, which yields

$$\left[\left(i\gamma^{\mu}\partial_{\mu}-m\right)\psi(x)\right]^{\dagger} = 0 \iff i\partial_{\mu}\psi^{\dagger}(x)\left(\gamma^{\mu}\right)^{\dagger}+m\psi^{\dagger}(x) = 0.$$
(1.151)

Taking advantage of the fact that

$$\gamma^{0}(\gamma^{\mu})^{\dagger}\gamma^{0} = \gamma^{\mu} \quad \Leftrightarrow \quad (\gamma^{\mu})^{\dagger} = \gamma^{0}\gamma^{\mu}\gamma^{0} \,, \tag{1.152}$$

we can multiply (1.151) by  $\gamma^0$  from right and write

$$0 = \left(i\partial_{\mu}\psi^{\dagger}(x)(\gamma^{\mu})^{\dagger} + m\psi^{\dagger}(x)\right)\gamma^{0}$$
$$= \left(i\partial_{\mu}\psi^{\dagger}(x)\gamma^{0}\gamma^{\mu} + m\psi^{\dagger}(x)\gamma^{0}\right)$$
$$= \left(i\partial_{\mu}\overline{\psi}(x)\gamma^{\mu} + m\overline{\psi}(x)\right)$$
$$= \overline{\psi}(x)\left(i\gamma^{\mu}\overleftarrow{\partial_{\mu}} + m\right).$$
(1.153)

From this we see that

$$\left(\partial_{\mu}\overline{\psi}(x)\right)\gamma^{\mu} = im\overline{\psi}. \qquad (1.154)$$

Plugging this into the (1.149) we obtain

$$\left(\partial_{\mu}\overline{\psi}(x)\right)\gamma^{\mu}\psi(x) + \overline{\psi}(x)\gamma^{\mu}\left(\partial_{\mu}\psi(x)\right)$$
  
=  $im\overline{\psi}(x)\psi(x) - im\overline{\psi}(x)\psi(x) = 0.$  (1.155)

So, current  $J^{\mu}$  is indeed conserved.

Note also that there is yet another possible candidate for probability current, namely the axial vector current

$$J^{\mu}(x) = \overline{\psi}(x)\gamma^{\mu}\gamma^{5}\psi(x). \qquad (1.156)$$

It can be, however, shown that in this case

$$\partial_{\mu}J^{\mu}(x) = 2im\overline{\psi}(x)\gamma^{5}\psi(x). \qquad (1.157)$$

So, this is conserved only when m = 0. Since in the standard model of particle physics there are no fundamental spin 1/2 particles that would have m = 0 (at observational energy scales), we will discard this type of current from our reasoning.

Let us now return back to the norm. Choose  $n^{\mu} = (1, 0, 0, 0)$ , then

$$\begin{aligned} (\psi,\psi) &= \int d^3 \boldsymbol{x} J_0(\boldsymbol{x}) = \int d^3 \boldsymbol{x} \overline{\psi}(\boldsymbol{x}) \gamma^0 \psi(\boldsymbol{x}) \\ &= \int d^3 \boldsymbol{x} \psi^{\dagger}(\boldsymbol{x}) \gamma^0 \gamma^0 \psi(\boldsymbol{x}) = \int d^3 \boldsymbol{x} \psi^{\dagger}(\boldsymbol{x}) \psi(\boldsymbol{x}) \ge 0. \end{aligned} (1.158)$$

From this we can see, that the would-be probability density  $\rho = J_0$  is positive definite. In addition, the norm is also time independent, since

$$-\underbrace{\frac{\partial}{\partial t} \int_{V} d^{3} \boldsymbol{x} \rho}_{\text{Change in total probability inside } V} = \int_{V} d^{3} \boldsymbol{x} \nabla \cdot \boldsymbol{J} = \underbrace{\int_{\partial V} d\boldsymbol{S} \cdot \boldsymbol{J}}_{\text{Flux of } \boldsymbol{J}} \to 0. \quad (1.159)$$

Here we used the same argument as in the Klein–Gordon particle case.

Finally, in order to see that the norm is relativistically invariant we can proceed as in the Klein–Gordon case, i.e., we first rewrite the norm as

$$||\psi||^{2} = \int d^{3}x \rho(x) = \int d^{4}x \underbrace{\delta(t_{0})}_{\frac{\partial}{\partial x^{0}} \theta(x_{0})} \rho(x)$$
$$= \int d^{4}x J^{\alpha} \frac{\partial}{\partial x^{\alpha}} \theta(n^{\beta} x_{\beta}). \qquad (1.160)$$

where  $n^{\mu} = (1, 0, 0, 0)$ . When  $||\psi||^2$  is Lorentz invariant it should equal to

$$||\widetilde{\psi}||^2 = \int d^4x J^{\alpha} \frac{\partial}{\partial x^{\alpha}} \theta(n^{\prime\beta} x_{\beta}), \qquad (1.161)$$

where  $n'^{\mu}$  is a unit time-like vector obtained from  $n^{\mu}$  via proper orthochronous Lorentz transformation.

Equivalence between  $||\tilde{\psi}||^2$  and  $|\psi||^2$  cane be explored by looking at their difference, i.e.

$$||\psi||^{2} - ||\widetilde{\psi}||^{2} = \int d^{4}x J^{\alpha} \frac{\partial}{\partial x^{\alpha}} \Big( \theta(n^{\beta}x_{\beta}) - \theta(n'^{\beta}x_{\beta}) \Big)$$
$$\overset{\partial_{\alpha}J^{\alpha} = 0}{\int} d^{4}x \frac{\partial}{\partial x^{\alpha}} \Big[ J^{\alpha} \{ \theta(n^{\beta}x_{\beta}) - \theta(n'^{\beta}x_{\beta}) \} \Big]$$
$$= \int dS_{\alpha} \Big[ J^{\alpha} \{ \theta(n^{\beta}x_{\beta}) - \theta(n'^{\beta}x_{\beta}) \} \Big]. \quad (1.162)$$

To show that this is zero it is enough to realize that:

- 1.  $J^{\alpha}$  vanishes if  $|\mathbf{x}| \to \infty$  with fixed *t*.
- 2.  $\theta(n^{\beta}x_{\beta}) \theta(n'^{\beta}x_{\beta})$  vanishes for  $|t| \to \infty$  with x fixed (for orthochronous transformations).

Hence, the difference (1.162) is zero and the norm is relativistically invariant. Again, we can define related scalar product as

$$(\psi_1,\psi_2) = \int dV n_\mu J^{\mu(1,2)}(x) , \qquad (1.163)$$

where  $J^{\mu(1,2)}(x) = \overline{\psi}_1(x)\gamma^{\mu}\psi_2(x)$ .

#### **Plane Wave Solutions of Dirac Equation**

We know that because  $\psi(x)$  satisfies Dirac equation, it must also satisfy Klein–Gordon equation. In particular, one may expect that wave functions of definite energy and momentum will be described by plane waves (i.e., de Broglie monochromatic waves) of the form

$$\begin{split} \psi_p^+(x) &= u(p)e^{-ipx} = u(p)e^{-i\omega_p t + i\boldsymbol{p}\cdot\boldsymbol{x}} \quad \text{(positive energy)}, \\ \psi_p^-(x) &= v(p)e^{ipx} = v(p)e^{i\omega_p t - i\boldsymbol{p}\cdot\boldsymbol{x}} \quad \text{(negative energy)}, \end{split} \tag{1.164}$$

where  $p_0 = \omega_p = \sqrt{p^2 + m^2} > 0$ . For the positive-energy plane wave  $i\partial_\mu \rightarrow p_\mu$  and given that  $(i\gamma^\mu\partial_\mu - m)\psi_p^+ = 0$  we obtain

$$(\gamma^{\mu}p_{\mu} - m)u(p) = 0 \iff (p - m)u(p) = 0,$$
 (1.165)

Similarly for the negative-energy solution we have

$$(\gamma^{\mu}p_{\mu} + m)v(p) = 0 \iff (p + m)v(p) = 0.$$
 (1.166)

In order to have a non-trivial solutions of Eqs. (1.165)-(1.166) we need to show that det (p - m) = 0 and det (p + m) = 0. To this end we use the

following trick:

$$det (\gamma^{\mu} p_{\mu} - m) = det \left(\gamma^{5} \gamma^{5} (\gamma^{\mu} p_{\mu} - m)\right)$$
$$= det \left(\gamma^{5} (\gamma^{\mu} p_{\mu} - m) \gamma^{5}\right)$$
$$= det \left(\left(-\gamma^{\mu} p_{\mu} - m\right) \gamma^{5} \gamma^{5}\right)$$
$$= det \left(\gamma^{\mu} p_{\mu} + m\right).$$
(1.167)

The second equation follows from property of determinants and the third from anticommutativity of  $\gamma^5$  with  $\gamma^{\mu}$ . From this we see that

$$\det \left[ \left( \gamma^{\mu} p_{\mu} - m \right) \left( \gamma^{\mu} p_{\mu} + m \right) \right] = \det \left( \gamma^{\nu} \gamma^{\mu} p_{\mu} p_{\nu} - m^{2} \right)$$
$$= \det^{2} \left( \gamma^{\mu} p_{\mu} \pm m \right) .$$
(1.168)

Using properties of  $\gamma$ -matrices we can further write that

$$\gamma^{\nu}\gamma^{\mu}p_{\mu}p_{\nu} - m^{2} = \frac{1}{2} \{\gamma^{\mu}, \gamma^{\nu}\} p_{\mu}p_{\nu} - m^{2} = p^{2} - m^{2}, \qquad (1.169)$$

and hence

$$\det^2 \left( \gamma^{\mu} p_{\mu} \pm m \right) = (p^2 - m^2)^4 = 0.$$
 (1.170)

Consequently, plane-wave solutions with non-trivial amplitudes are solutions of Dirac's equation.

#### **Positive Energy Solutions**

From the Dirac representation of  $\gamma$ -matrices we find that

$$\left(\gamma^{\mu}p_{\mu}-m\right) = \begin{pmatrix} (E-m)\mathbf{1} & -\boldsymbol{\sigma}\cdot\boldsymbol{p} \\ \boldsymbol{\sigma}\cdot\boldsymbol{p} & -(E+m)\mathbf{1} \end{pmatrix}.$$
 (1.171)

Consider u(p) in the form

$$u(p) = \begin{pmatrix} \chi \\ \varphi \end{pmatrix}, \qquad (1.172)$$

where  $\chi$  and  $\varphi$  are both 2-component columns. From this we can rewrite equation (1.165) as a system of two coupled equations

$$(E-m)\chi - \boldsymbol{\sigma} \cdot \boldsymbol{p}\varphi = 0, \qquad (1.173)$$

$$\boldsymbol{\sigma} \cdot \boldsymbol{p} \chi - (E+m)\varphi = 0. \qquad (1.174)$$

The *on-mass-shell* condition  $p^2 = m^2$ , in fact, ensures, that these two equations are equivalent. Indeed, multiplying (1.173) by (E + m) we obtain

$$\underbrace{(E^2 - m^2)}_{\boldsymbol{p}^2} \chi - \boldsymbol{\sigma} \cdot \boldsymbol{p}(E + m)\varphi = 0. \qquad (1.175)$$
Similarly, by multiplying (1.174) from left by  $\sigma \cdot p$  we get

$$\sigma^{i}\sigma^{j}p_{i}p_{j}\chi - \boldsymbol{\sigma}\cdot\boldsymbol{p}(E+m)\varphi = 0. \qquad (1.176)$$

Using the fact that  $\sigma^i \sigma^j p_i p_j$  can be rewritten as  $\frac{1}{2} \{\sigma^i, \sigma^j\} p_i p_j = \delta^{ij} p_i p_j = p^2$  we get that those two equations are indeed equivalent and any of the two can be used. In particular, from the second equation we obtain that

$$\varphi = \frac{\boldsymbol{\sigma} \cdot \boldsymbol{p}}{E+m} \chi \,, \tag{1.177}$$

which implies that

$$u(p) \propto \begin{pmatrix} \chi \\ \frac{\boldsymbol{\sigma} \cdot \boldsymbol{p}}{E+m} \chi \end{pmatrix}$$
 (1.178)

For our future convenience we fix the normalization of u(p) so that

$$u(p) = \sqrt{E+m} \begin{pmatrix} \chi \\ \frac{\sigma \cdot p}{E+m} \chi \end{pmatrix}.$$
(1.179)

**Other Normalizations** 

Often the normalization is chosen differently, namely

$$u(p) = \sqrt{\frac{E+m}{2m}} \begin{pmatrix} \chi \\ \frac{\boldsymbol{\sigma} \cdot \boldsymbol{p}}{E+m} \chi \end{pmatrix} = \begin{pmatrix} \sqrt{\frac{E+m}{2m}} \chi \\ \frac{\boldsymbol{\sigma} \cdot \boldsymbol{p}}{\sqrt{2m(E+m)}} \chi \end{pmatrix}.$$

This gives nicer normalization for  $\overline{u}u$  and  $\overline{v}v$ .

There is another, more physical way of solving (p - m) u(p) = 0 and (p + m) v(p) = 0 equations. Let assume that  $m \neq 0$ . In the rest frame of the particle  $p^{\mu} = (m, 0)$ , which implies that the aforementioned Dirac equations reduce to

$$\left(\gamma^{0} - \mathbb{1}\right) u(m, \mathbf{0}) = 0,$$
 (1.180)

$$\left(\gamma^0 + \mathbb{1}\right) v(m, \mathbf{0}) = 0.$$
(1.181)

There are clearly 2 linearly independent solutions for both u and v, namely

$$\begin{aligned} u^{(1)}(m,\mathbf{0}) &= \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix}, \quad u^{(2)}(m,\mathbf{0}) &= \begin{pmatrix} 0\\1\\0\\0 \end{pmatrix}, \\ v^{(1)}(m,\mathbf{0}) &= \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix}, \quad v^{(2)}(m,\mathbf{0}) &= \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix}. \end{aligned}$$
(1.182)

We could now boost these solutions from a rest up to a velocity  $|\nu| = \frac{|p|}{p_0}$  by a pure Lorentz transformation  $S(\Lambda) = e^{-\frac{i}{4}\sigma_{\mu\nu}\omega^{\mu\nu}}$ .

**3-velocity in relativity** Note that  $p^{\mu} = \left(\frac{E}{c}, p\right) = \frac{m_0}{\sqrt{1 - \frac{v^2}{c^2}}}(c, v)$ . So, by setting c = 1 we have that  $|v| = \frac{|p|}{p_0}$ .

Inner workings of this will be explicitly seen in section that deals with boost transformations.

There exists also a simpler passage to the solution that employs a trivial fact that

$$(p - m) (p + m) = p^2 - m^2 = (p + m) (p - m) = 0.$$
 (1.183)

So, in particular

$$(p - m) (p + m) u^{(\lambda)} = 0, \quad \lambda = 1, 2.$$
 (1.184)

This implies that the positive-energy solution is of the form

$$(p + m) u^{(\lambda)}(m, \mathbf{0}) = \begin{pmatrix} E + m & -\boldsymbol{\sigma} \cdot \boldsymbol{p} \\ \boldsymbol{\sigma} \cdot \boldsymbol{p} & -(E - m) \end{pmatrix} u^{(\lambda)}(m, \mathbf{0})$$
$$= \begin{pmatrix} (E + m) \chi^{(\lambda)} \\ \boldsymbol{\sigma} \cdot \boldsymbol{p} \chi^{(\lambda)} \end{pmatrix}.$$
(1.185)

Here we employed the fact that

$$u^{(\lambda)}(m,\mathbf{0}) = \begin{pmatrix} \chi^{(\lambda)}(m,\mathbf{0}) \\ 0 \\ 0 \end{pmatrix}, \qquad (1.186)$$

and that  $\chi^{(\lambda)}$  is either  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$  or  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ .

Negative energy solution is obtained similarly, namely it is of the form

$$(\not p - m) v^{(\lambda)}(m, \mathbf{0}) = \begin{pmatrix} E - m & -\boldsymbol{\sigma} \cdot \boldsymbol{p} \\ \boldsymbol{\sigma} \cdot \boldsymbol{p} & -(E + m) \end{pmatrix} v^{(\lambda)}(m, \mathbf{0})$$
$$= \begin{pmatrix} -\boldsymbol{\sigma} \cdot \boldsymbol{p} \chi^{(\lambda)} \\ -(E + m) \chi^{(\lambda)} \end{pmatrix}.$$
(1.187)

Where in analogy with positive energy solution, we write

$$v^{(\lambda)}(m,\mathbf{0}) = \begin{pmatrix} 0\\ 0\\ \chi^{(\lambda)}(m,\mathbf{0}) \end{pmatrix}, \qquad (1.188)$$

and  $\chi^{(\lambda)}$  is again  $\begin{pmatrix} 1 \\ 0 \end{pmatrix}$  or  $\begin{pmatrix} 0 \\ 1 \end{pmatrix}$ . Relation with our former normalization is

obtained when we write

$$u^{(\lambda)}(p) = \frac{\not p + m}{\sqrt{E + m}} u^{(\lambda)}(m, \mathbf{0}),$$
  
$$v^{(\lambda)}(p) = \frac{-\not p + m}{\sqrt{E + m}} v^{(\lambda)}(m, \mathbf{0}). \qquad (1.189)$$

#### Non-relativistic limit and relation to the Schrödinger equation

Recall that positive and negative energy solutions to the massive Dirac equation have the form

$$u_{\lambda} = \sqrt{E+m} \begin{pmatrix} \chi_{\lambda} \\ \frac{\sigma \cdot p}{E+m} \chi_{\lambda} \end{pmatrix} \equiv \begin{pmatrix} u_L \\ u_S \end{pmatrix}.$$
(1.190)

Note that  $u_S = \frac{\sigma \cdot p}{E+m} u_L$ . Similarly for negative energy solution we can write

$$v_{\lambda} = \sqrt{E+m} \begin{pmatrix} \frac{\sigma \cdot p}{E+m} \varphi_{\lambda} \\ \varphi_{\lambda} \end{pmatrix} \equiv \begin{pmatrix} v_{S} \\ v_{L} \end{pmatrix}, \qquad (1.191)$$

and  $v_S = \frac{\sigma \cdot p}{E+m} v_L$ . In the non-relativistic limit  $|\mathbf{p}| \ll m$  and so  $u_S \ll u_L$  and  $v_S \ll v_L$ . The subscript "*S*" refers to the so-called *small component* and the subscript "*L*" to the *large component*.

The positive energy solutions satisfy

$$\begin{pmatrix} m\mathbf{1} & \boldsymbol{\sigma} \cdot \boldsymbol{p} \\ \boldsymbol{\sigma} \cdot \boldsymbol{p} & -m\mathbf{1} \end{pmatrix} \begin{pmatrix} u_L \\ u_S \end{pmatrix} = E \begin{pmatrix} u_L \\ u_S \end{pmatrix}.$$
(1.192)

This equation can be rewritten as

$$\boldsymbol{\sigma} \cdot \boldsymbol{p} \, \boldsymbol{u}_S = (E - m) \boldsymbol{u}_L \,, \tag{1.193}$$

$$\boldsymbol{\sigma} \cdot \boldsymbol{p} \, \boldsymbol{u}_L \; = \; (E+m) \boldsymbol{u}_S \, . \tag{1.194}$$

By substituting (1.194) to (1.193) we get

$$\frac{(\boldsymbol{\sigma} \cdot \boldsymbol{p})(\boldsymbol{\sigma} \cdot \boldsymbol{p})}{E+m} u_L = (E-m)u_L.$$
(1.195)

We now use the fact that  $(\sigma \cdot p)(\sigma \cdot p) = p^2$  and that  $|p| \ll m$  implies  $E \approx m$ . With this we can rewrite (1.195) as

$$\frac{p^2}{2m}u_L = (E-m)u_L = E_{NR}u_L, \qquad (1.196)$$

where  $E_{NR}$  is the non-relativist energy spectrum. This is the usual Schrödinger equation for a free non-relativistic particle. To understand the 2-component nature of  $u_L$  we need to understand better how u(p) transforms under the Lorentz group.

## **Applications of Lorentz Transformations on Dirac Wave Functions**

We will begin with *rotations of Dirac wave functions*. We know that that the group of rotations {*R*} is a subgroup of the group of Lorentz transformations {*L*}. We have seen that a generic element of the Lorentz group has the form  $L = e^{-\frac{i}{4}M^{\mu\nu}\omega_{\mu\nu}}$ . In particular, generators of rotations are described by  $M^{ij}$  (*i*, *j* = 1, 2, 3). Connection between  $M^{ij}$  and  $J_i$  is established via relation

$$J_i = \frac{1}{4} \varepsilon_{ijk} M^{jk}$$
 or equivalently  $M^{jk} = 2\varepsilon^{jki} J_i$ . (1.197)

In particular, when  $M^{\mu\nu}$  acts on 4-vectors (i.e., it is in a fundamental representation) then

$$(M^{\mu\nu})^{\rho}{}_{\tau} = 2i \left[ \eta^{\mu\rho} \eta^{\nu}{}_{\tau} - \eta^{\nu\rho} \eta^{\mu}{}_{\tau} \right] .$$
(1.198)

This gives us

$$\left(\boldsymbol{J}_{i}\right)^{\rho}{}_{\tau} = \frac{i}{2}\varepsilon_{ijk}\left[\eta^{\rho j}\eta^{k}{}_{\tau} - \eta^{\rho k}\eta^{j}{}_{\tau}\right].$$
(1.199)

So, for instance, for a third component we can write

$$\left(\boldsymbol{J}_{3}\right)^{\rho}{}_{\tau} = \frac{i}{2}\varepsilon_{3jk}\left[\eta^{\rho j}\eta^{k}{}_{\tau} - \eta^{\rho k}\eta^{j}{}_{\tau}\right].$$
(1.200)

From this we see, that *j* has can be either 1 or 2, and *k* either 2 or 1, respectively. Hence, non-trivial contributions to  $(J_3)^{\rho}_{\tau}$  come only from components  $\rho = 1, 2, \tau = 2, 1$ . Namely

$$(\boldsymbol{J}_{3})^{1}{}_{2} = \frac{i}{2} \varepsilon_{312} \eta^{11} \eta_{2}^{2} - \frac{i}{2} \varepsilon_{321} \eta^{11} \eta_{2}^{2} = -i,$$
  

$$(\boldsymbol{J}_{3})^{2}{}_{1} = \frac{i}{2} \varepsilon_{321} \eta^{22} \eta_{1}^{1} - \frac{i}{2} \varepsilon_{312} \eta^{22} \eta_{1}^{1} = i.$$
 (1.201)

Thus we can finally write that  $J_3$  has an explicit form

$$\boldsymbol{J}_{3} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & -i & 0 \\ 0 & i & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}.$$
 (1.202)

In a similar way we obtain

It is easy to see that the generators  $J_i$  can be written in the compact form

$$(\boldsymbol{J}_i)_{jk} = -i \left( \begin{array}{c|c} 0 & 0 \\ \hline 0 & \varepsilon_{ijk} \end{array} \right), \qquad (1.204)$$

Recall that  $[J_i, J_j] = i\varepsilon_{ijk}J_k$  — i.e., they close a familiar algebra of rotations  $SU(2) \sim SO(3)$ .

Upper index labels rows, while the lower one labels columns.

so they represent angular momentum generators in adjoint representation (as their 3D counterparts).

On the other hand, we know that a general element of the subgroup of rotations has the form

$$R = e^{-\frac{i}{4}\omega_{ij}M^{ij}} = e^{-\frac{i}{2}\varepsilon^{ijk}\omega_{ij}J_k} = e^{-i\theta^k J_k}.$$
 (1.205)

Here we have defined  $\theta^k = \frac{1}{2} \varepsilon^{ijk} \omega_{ij}$ . So, for instance the rotation around *z*-axis should have the form

$$\boldsymbol{R}_3 = e^{-i\boldsymbol{\theta}\boldsymbol{J}_3}. \tag{1.206}$$

This can be computed explicitly. Let us first denote the central  $2 \times 2$  matrix in  $J_{3}$ , i.e.

$$\left(\begin{array}{cc} 0 & -i\\ i & 0 \end{array}\right), \tag{1.207}$$

as  $\tilde{J}_3$ . Using the fact that  $\tilde{J}_3$  is *involutory matrix*, i.e.,  $(\tilde{J}_3)^2 = 1$ , we can write

$$e^{-i\theta J_{3}} = \begin{pmatrix} 1 & \mathbf{0} & \mathbf{0} & 0 \\ \mathbf{0} & \sum_{n=0}^{\infty} \frac{(-i\theta)^{n}}{n!} \tilde{J}_{3}^{n} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & \mathbf{0} & \mathbf{0} & 0 \\ \mathbf{0} & \sum_{n=0}^{\infty} \frac{(-1)^{n}}{2n!} (\theta)^{2n} \mathbf{1}_{2\times 2} - i \sum_{n=0}^{\infty} \frac{(-1)^{n}}{(2n+1)!} (\theta)^{2n+1} \tilde{J}_{3} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & \mathbf{0} & \mathbf{0} & 0 \\ \mathbf{0} & \cos \theta \mathbf{1}_{2\times 2} - i \sin \theta \tilde{J}_{3} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} & 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 & 0 & 0 & 0 \\ \mathbf{0} & \cos \theta - \sin \theta & 0 \\ \mathbf{0} & \sin \theta & \cos \theta & 0 \\ \mathbf{0} & \mathbf{0} & 1 \end{pmatrix}, \qquad (1.208)$$

which describes a rotation in the x - y plane (i.e., rotation around *z*-axis) by angle  $\theta$ . Along the same lines one can show that a rotation along arbitrary axis specified by the unit 3-vector **n** is done by

$$\boldsymbol{R} = e^{-i\theta^i \boldsymbol{J}_i} \,. \tag{1.209}$$

Note that we can equivalently write that

$$\boldsymbol{\theta}^{i}\boldsymbol{J}_{i} = \boldsymbol{\theta}\boldsymbol{n}^{i}\boldsymbol{J}_{i}, \qquad (1.210)$$

where  $\theta$  is rotation angle around axis *n*. Since  $\theta$  corresponds to respective components of the rotational angle we have succeeded to relate the abstract parameters  $\omega_{ij}$  with the physical parameters  $\theta_i$  (cf.  $\theta^k = \frac{1}{2} \varepsilon^{ijk} \omega_{ij}$ ).

The corresponding representation of rotations that acts on Dirac wave functions can be constructed from generators  $\sigma^{ij}$  by realizing the

One can indeed check that 
$$J_k = i \frac{\partial R}{\partial \theta^k} \Big|_{\theta=0}$$
.

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following parallelism

$$L = e^{-\frac{i}{4}M^{\mu\nu}\omega_{\mu\nu}} \leftrightarrow S(L) = e^{-\frac{i}{4}\sigma^{\mu\nu}\omega_{\mu\nu}},$$
  
$$R = e^{-\frac{i}{4}M^{ij}\omega_{ij}} = e^{-i\theta n^{i}J_{i}} \leftrightarrow S(R) = e^{-\frac{i}{4}\sigma^{ij}\omega_{ij}} = e^{-i\theta n^{i}\hat{\sigma}_{i}}.$$
 (1.211)

Here  $\hat{\sigma}_i = \frac{1}{4} \varepsilon_{ijk} \sigma^{jk} \Leftrightarrow \sigma^{jk} = 2 \varepsilon^{ijk} \hat{\sigma}_i$ . Let us find explicit form of  $\hat{\sigma}_i$ . Starting from the definition of  $\sigma^{ij}$ , we get in Dirac's representation

$$\sigma^{ij} = \frac{i}{2} [\gamma^{i}, \gamma^{j}] = i\gamma^{i}\gamma^{j}$$

$$= i \begin{pmatrix} 0 & \sigma^{i} \\ -\sigma^{i} & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma^{j} \\ -\sigma^{j} & 0 \end{pmatrix} = i \begin{pmatrix} -\sigma^{i}\sigma^{j} & 0 \\ 0 & -\sigma^{i}\sigma^{j} \end{pmatrix}$$

$$= \begin{pmatrix} \sigma_{k} & 0 \\ 0 & \sigma_{k} \end{pmatrix} \varepsilon^{ijk} . \qquad (1.212)$$

Consequently,  $\hat{\sigma}_k$  reads

$$\hat{\sigma}_{k} = \frac{1}{4} \varepsilon_{klm} \sigma^{lm} = \frac{1}{4} \varepsilon_{klm} \varepsilon^{lmp} \begin{pmatrix} \sigma_{p} & 0\\ 0 & \sigma_{p} \end{pmatrix}$$

$$= \frac{1}{4} \varepsilon_{lmk} \varepsilon^{lmp} \begin{pmatrix} \sigma_{p} & 0\\ 0 & \sigma_{p} \end{pmatrix}$$

$$= \frac{1}{4} (\delta_{m}^{m} \delta_{k}^{p} - \delta_{m}^{p} \delta_{k}^{m}) \begin{pmatrix} \sigma_{p} & 0\\ 0 & \sigma_{p} \end{pmatrix}$$

$$= \frac{1}{2} \begin{pmatrix} \sigma_{k} & 0\\ 0 & \sigma_{k} \end{pmatrix}. \qquad (1.213)$$

#### Algebra of generators $\hat{\sigma}_k$

Taking commutator

$$[\hat{\boldsymbol{\sigma}}_k, \hat{\boldsymbol{\sigma}}_l] = \begin{pmatrix} \frac{1}{2} [\sigma_k, \sigma_l] & 0\\ 0 & \frac{1}{2} [\sigma_k, \sigma_l] \end{pmatrix} = \frac{i}{2} \varepsilon_{klm} \begin{pmatrix} \sigma_m & 0\\ 0 & \sigma_m \end{pmatrix} = i \varepsilon_{klm} \hat{\boldsymbol{\sigma}}_m.$$

Hence  $\hat{\sigma}_i$  are correct generators of rotations in Dirac's space of wave functions (so-called *bispinor space*).

By denoting

$$2\hat{\sigma}_k = \Sigma_k = \begin{pmatrix} \sigma_k & 0\\ 0 & \sigma_k \end{pmatrix}, \qquad (1.214)$$

we obtain that

$$S(\mathbf{R}) = e^{-\frac{i}{2}\theta \mathbf{n}^{k}\Sigma_{k}} = \begin{pmatrix} e^{-\frac{i}{2}\theta \mathbf{n}_{k}\sigma_{k}} & 0\\ 0 & e^{-\frac{i}{2}\theta \mathbf{n}_{k}\sigma_{k}} \end{pmatrix}.$$
 (1.215)

Consider now action of  $S(\mathbf{R})$  on u(p):

$$S(\mathbf{R})u(p) = \begin{pmatrix} e^{-\frac{i}{2}\theta\mathbf{n}_{k}\sigma_{k}} & 0\\ 0 & e^{-\frac{i}{2}\theta\mathbf{n}_{k}\sigma_{k}} \end{pmatrix} u(p)$$
$$= \sqrt{E+m} \begin{pmatrix} e^{-\frac{i}{2}\theta\mathbf{n}_{k}\sigma_{k}} & 0\\ 0 & e^{-\frac{i}{2}\theta\mathbf{n}_{k}\sigma_{k}} \end{pmatrix} \begin{pmatrix} \chi\\ \frac{\sigma \cdot p}{E+m} \chi \end{pmatrix}$$
$$= \sqrt{E+m} \begin{pmatrix} e^{-\frac{i}{2}\theta\mathbf{n} \cdot \sigma} \chi\\ \frac{e^{-\frac{i}{2}\theta\mathbf{n} \cdot \sigma} \mathbf{y} e^{\frac{i}{2}\theta\mathbf{n} \cdot \sigma}}{E+m} e^{-\frac{i}{2}\theta\mathbf{n} \cdot \sigma} \chi \end{pmatrix}. \quad (1.216)$$

Define  $\chi_{\mathbf{R}} = e^{-\frac{i}{2}\theta \mathbf{n} \cdot \boldsymbol{\sigma}} \chi$ , where  $\frac{\sigma}{2}$  are generators of rotations in representation with spin 1/2. So,  $\chi$  can be identified with a 2-component spinor.

We can now use the following identity (it can be easily check to the leading order in  $\theta$ )

$$e^{-\frac{i}{2}\theta \boldsymbol{n}\cdot\boldsymbol{\sigma}}\boldsymbol{\sigma}\cdot\boldsymbol{p}e^{\frac{i}{2}\theta \boldsymbol{n}\cdot\boldsymbol{\sigma}} = \boldsymbol{\sigma}e^{-i\theta \boldsymbol{n}\cdot\boldsymbol{J}}\cdot\boldsymbol{p}.$$
(1.217)

(cf. with the similar relation  $S^{-1}(L)\gamma^{\mu}S(L) = L^{\mu}_{\nu}\gamma^{\nu} = \gamma^{\nu}L^{\mu}_{\nu}$ ). From this we finally get the rotated Dirac's wave function in the form

$$S(\mathbf{R})u(p) = \sqrt{E+m} \begin{pmatrix} \chi_{\mathbf{R}} \\ \frac{\sigma \cdot p_{\mathbf{R}}}{E+m} \chi_{\mathbf{R}} \end{pmatrix} = u_{\mathbf{R}}(p_{\mathbf{R}}).$$
(1.218)

We thus see that  $u_R$  is constructed from the rotated spinor  $\chi_R$  and  $p_R$  is the rotated 4-momentum, i.e.,  $p_R = (p_0, p_R)$ .

Let us now introduce Pauli spinors  $\chi_{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$  and  $\chi_{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$  and denote them generally as  $\chi_{\lambda}$  with  $\lambda = \pm \frac{1}{2}$ . Then

$$u_{\lambda}(p) = \sqrt{E+m} \begin{pmatrix} \chi_{\lambda} \\ \frac{\sigma \cdot p}{E+m} \chi_{\lambda} \end{pmatrix}, \qquad (1.219)$$

and  $\lambda = \pm \frac{1}{2}$  (as seen in the box) has a meaning of the "third component of spin".

#### Action of Rotation Generators on Free Solutions of Dirac's Equation in the Rest Frame

Let us look what happens, when we apply generators of rotations (angular momentum operators) on free solutions of Dirac equation in the rest frame. We know that these solutions have general form

$$\begin{split} \psi_{\lambda}^{+}(x) &= \sqrt{2m} \begin{pmatrix} \chi_{\lambda} \\ 0 \end{pmatrix} \frac{e^{-ik_{0}t + i\boldsymbol{k}\cdot\boldsymbol{x}}}{\sqrt{2\pi}^{3}} , \\ \psi_{\lambda}^{-}(x) &= \sqrt{2m} \begin{pmatrix} 0 \\ \chi_{\lambda} \end{pmatrix} \frac{e^{ik_{0}t - i\boldsymbol{k}\cdot\boldsymbol{x}}}{\sqrt{2\pi}^{3}} , \end{split}$$

with  $\mathbf{k} \cdot \mathbf{x}$  being zero in the rest frame and  $k_0 = m$ . We also know

2-component wave function that transforms under rotations as  $\chi_{\mathbf{R}} = e^{-\frac{i}{2}\theta \mathbf{n} \cdot \boldsymbol{\sigma}} \chi$ , is known in quantum mechanics as *Pauli spinor*. In mathematics this is better known as *Weyl spinor*.

 $oldsymbol{J}_i \ \leftrightarrow \ \hat{oldsymbol{\sigma}} \ = \ rac{1}{2} egin{pmatrix} \sigma_i & 0 \ 0 & \sigma_i \end{pmatrix}$  ,

and in particular

that

$$\sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix},$$

which leads to

$$J_{3}\psi_{\frac{1}{2}}^{+} = \frac{1}{2}\psi_{\frac{1}{2}}^{+}, \quad J_{3}\psi_{-\frac{1}{2}}^{+} = -\frac{1}{2}\psi_{-\frac{1}{2}}^{+},$$
$$J_{3}\psi_{\frac{1}{2}}^{-} = \frac{1}{2}\psi_{\frac{1}{2}}^{-}, \quad J_{3}\psi_{-\frac{1}{2}}^{-} = -\frac{1}{2}\psi_{-\frac{1}{2}}^{-}.$$

These relations imply that Dirac's bispinors describe particle with spin 1/2.

# 1.8 Lorentz Boosts and Dirac Wave Function

Lorentz boost in *x* direction can be written as

$$t' = \gamma(t - vx) \iff x'_{0} = \gamma(x_{0} - \beta x),$$
  

$$x' = \gamma(x - vt) \iff x' = \gamma(x - \beta x_{0}),$$
  

$$y' = y,$$
  

$$z' = z,$$
  
(1.220)

where  $v = \beta$  and  $-1 < \beta < 1$  (note that we use the notation c = 1).

The Lorentz transformations are often also written in a way that resembles rotations in 3D using hyperbolic functions. This is possible, because  $\beta$  and  $\gamma$  satisfy identity

$$\gamma^2 - \gamma^2 \beta^2 = \gamma^2 (1 - \beta^2) = 1, \qquad (1.221)$$

which allows us to set  $\gamma \equiv \cosh \zeta$  and  $\gamma \beta \equiv \sinh \zeta$ . With this, we can rewrite (1.220) equivalently as

$$x'_{0} = x_{0} \cosh \zeta - x \sinh \zeta,$$
  

$$x' = x \cosh \zeta - x_{0} \sinh \zeta,$$
  

$$y' = y,$$
  

$$z' = z.$$
(1.222)

In this connection we note that

$$\cosh \zeta = \gamma = \frac{1}{\sqrt{1-\beta^2}} = \frac{1}{\sqrt{1-\tanh^2 \zeta}},$$

$$\tanh \zeta = \frac{\sinh \zeta}{\cosh \zeta} = \beta \implies \zeta = \tanh^{-1} \beta. \quad (1.223)$$

Since  $\beta \in (-1, 1)$ , we get that  $\zeta \in (-\infty, \infty)$ . The new variable  $\zeta$  is known as *rapidity*.

Similar equations can also be written for boost in z direction

$$x'_{0} = x_{0} \cosh \zeta - z \sinh \zeta,$$
  

$$x' = x,$$
  

$$y' = y,$$
  

$$z' = z \cosh \zeta - x_{0} \sinh \zeta,$$
 (1.224)

and similarly for *y* direction.

Aforestated boost transformations can be written in terms of boost matrices as

$$L_{x} = \begin{pmatrix} \cosh \zeta & -\sinh \zeta & 0 & 0 \\ -\sinh \zeta & \cosh \zeta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$
$$L_{z} = \begin{pmatrix} \cosh \zeta & 0 & 0 & -\sinh \zeta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ -\sinh \zeta & 0 & 0 & \cosh \zeta \end{pmatrix}, \qquad (1.225)$$

and similarly for  $L_{y}$ .

Consider now a particle with mass *m* in its rest frame. In such a case it has a four-momentum  $p^{\mu} = (m, 0, 0, 0)$ . Let us now boost the particle to the second frame, which moves with velocity *v* in the -z-direction of the first (i.e., -v velocity in the positive *z*-axis direction). Then in the new frame the *z* momentum of the particle will appear increased. In particular, we can write this boost transformation from the rest frame in the form

$$p' = L_z p = \begin{pmatrix} \cosh \zeta & 0 & 0 & \sinh \zeta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \sinh \zeta & 0 & 0 & \cosh \zeta \end{pmatrix} \begin{pmatrix} m \\ 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} E \\ 0 \\ 0 \\ q \end{pmatrix}, \quad (1.226)$$

where  $E = m \cosh \zeta = m\gamma$  and  $q = m \sinh \zeta = mv\gamma$  (relativistic threemomentum). So, in this case,  $\tanh \zeta = q/E = \beta$ .

If  $\zeta$  is infinitesimal (i.e.,  $|\zeta| \ll 1$ ), we can write the boost matrix in z direction as

$$\boldsymbol{L}_{z} \approx \begin{pmatrix} 1 & 0 & 0 & \zeta \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ \zeta & 0 & 0 & 1 \end{pmatrix} = \boldsymbol{1} + \zeta \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$
(1.227)

Rapidity is a standard parameter that quantifies relativistic velocities in particle physics. In 1D motion, rapidities are additive whereas velocities must be combined via Einstein's velocity-addition formula. At the same time, we can use Eq. (1.108) and write

$$L_{z} \approx \mathbf{1} - \frac{i}{4}\omega_{\mu\nu}M^{\mu\nu} = \mathbf{1} - \frac{i}{4}(\omega_{03}M^{03} + \omega_{30}M^{30})$$
$$= \mathbf{1} - \frac{i}{2}\omega_{03}M^{03}. \qquad (1.228)$$

Here we used the fact that  $\omega_{\mu\nu} = 0$  except for boost in 3rd direction where  $\omega_{03} = -\omega_{30} \neq 0$ . By using the relation  $\mathbf{K}^i = \frac{1}{2}\mathbf{M}^{0i}$  we can identify  $\omega_{03}$  with  $\zeta$  and

$$\boldsymbol{K}^{3} = i \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}, \quad \boldsymbol{M}^{03} = 2i \begin{pmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \end{pmatrix}.$$
(1.229)

As an independent check we can now go back to finite transformations, i.e.

$$L_{z} = \exp\left(-\frac{i}{2}\omega_{03}M^{03}\right) = \exp\left\{\zeta \begin{pmatrix} 0 & 0 & 0 & 1\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0\\ 1 & 0 & 0 & 0 \end{pmatrix}\right\}$$
$$= \begin{pmatrix} \cosh\zeta & 0 & 0 & \sinh\zeta\\ 0 & 1 & 0 & 0\\ 0 & 0 & 1 & 0\\ \sinh\zeta & 0 & 0 & \cosh\zeta \end{pmatrix}, \qquad (1.230)$$

where in the last step we used the fact that the matrix  $\begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}$  is involutive. This result indeed coincides with  $L_z$  given in (1.225), with  $v \rightarrow -v$ .

In the bispinor space the ensuing matrix responsible for boosts is given by

$$S(L) = \exp\left\{-\frac{i}{2}\omega_{0i}\sigma^{0i}\right\}.$$
 (1.231)

In particular, in the *z* direction we have

$$S(L_z) = \exp\left\{-\frac{i}{2}\zeta\sigma^{03}\right\},\qquad(1.232)$$

where  $\sigma^{03} = \frac{i}{2} [\gamma^0, \gamma^3] = i \gamma^0 \gamma^3$ , so

$$S(\boldsymbol{L}_{z}) = \exp\left\{-\frac{i}{2}\zeta i\gamma^{0}\gamma^{3}\right\} = \exp\left\{\frac{\zeta}{2}\gamma^{0}\gamma^{3}\right\}.$$
 (1.233)

Let us now compute the explicit form of  $S(L_z)$ . Firstly, we observe that  $(\gamma^0 \gamma^3)^2 = \gamma^0 \gamma^3 \gamma^0 \gamma^3 = -\gamma^0 \gamma^0 \gamma^3 \gamma^3 = -\mathbf{1}(-\mathbf{1}) = \mathbf{1}$ , which implies that  $\gamma^0 \gamma^3$  is an involutive matrix. By using the identity

$$e^{xN} = (\cosh x)\mathbf{1} + (\sinh x)N$$
, (1.234)

Note that  $M^{03}$  is consistent with the defining formula (1.84).

Note that the matrix  $S(L_z)$  is nonunitary. This is consequence of the fact that there are no finite dimensional unitary representations for non-compact groups (e.g. Lorentz group) of which boosts are examples. which is valid for any involutive matrix N, we obtain

$$S(L_z) = \cosh \frac{\zeta}{2} + \gamma^0 \gamma^3 \sinh \frac{\zeta}{2}. \qquad (1.235)$$

Secondly, using hyperbolic half-argument formulas, one can write

$$\cosh \frac{\zeta}{2} = \sqrt{\frac{\cosh \zeta + 1}{2}} = \sqrt{\frac{E/m + 1}{2}} = \sqrt{\frac{E+m}{2m}}, \quad (1.236)$$

and

$$\sinh \frac{\zeta}{2} = \sqrt{\frac{\cosh \zeta - 1}{2}} = \sqrt{\frac{E - m}{2m}} = \sqrt{\frac{E^2 - m^2}{2m(E + m)}}$$
$$= \sqrt{\frac{q^2}{2m(E + m)}}, \qquad (1.237)$$

since  $\cosh \zeta = \gamma$  and  $E = \gamma m$  we have that  $\cosh \zeta = E/m$ . Here *m* is rest mass and *q* relativistic three-momentum. From (1.236) and (1.237) we can read off that

$$S(L_z) = \sqrt{\frac{E+m}{2m}} \left[ \mathbbm{1} + \frac{q}{E+m} \gamma^0 \gamma^3 \right].$$
(1.238)

Thirdly, we observe that in Dirac's representation

$$\gamma^{0}\gamma^{3} = (\sigma^{3} \otimes \mathbb{1})(i\sigma^{2} \otimes \sigma^{3}) = (\sigma^{3}i\sigma^{2} \otimes \sigma^{3}) = \begin{pmatrix} \mathbf{0} & \sigma^{3} \\ \sigma^{3} & \mathbf{0} \end{pmatrix}.$$
 (1.239)

Consequently, we can write the bispinor representation of boost transformation in *z*-direction as

$$S(L_z) = \sqrt{\frac{E+m}{2m}} \begin{pmatrix} \mathbb{1} & \frac{q}{E+m}\sigma^3\\ \frac{q}{E+m}\sigma^3 & \mathbb{1} \end{pmatrix}.$$
 (1.240)

This result might be generalized to boost in general 3-velocity v = q/E direction. Ensuing transformation takes the form

$$S(L) = \sqrt{\frac{E+m}{2m}} \begin{pmatrix} \mathbb{1} & \frac{q}{E+m}\sigma \\ \frac{q}{E+m}\sigma & \mathbb{1} \end{pmatrix}.$$
 (1.241)

As an example, we can consider a particle in the rest frame, i.e., with four-momentum  $\bar{p}^{\mu} = \binom{m}{0}$ . In this case the Dirac spinor is

$$u_{\lambda}(\bar{p}) = \sqrt{2m} \begin{pmatrix} \chi_{\lambda} \\ 0 \end{pmatrix}.$$
 (1.242)

When boosting system to a frame with velocity -v in *z*-direction we get

$$p = \mathbf{L}_{z}\bar{p} = \begin{pmatrix} E\\0\\0\\q \end{pmatrix}, \qquad (1.243)$$

Note that in bispinor representation S(L), the arguments of hyperbolic sine and cosine are  $\zeta/2$  whereas in fundamental representation L, the arguments are just  $\zeta$ .

and

$$u_{\lambda}(p) = S(L_{z})u_{\lambda}(\bar{p}) = \sqrt{\frac{E+m}{2m}} \begin{pmatrix} \mathbf{1} & \frac{q\sigma^{3}}{E+m} \\ \frac{q\sigma^{3}}{E+m} & \mathbf{1} \end{pmatrix} \sqrt{2m} \begin{pmatrix} \chi_{\lambda} \\ 0 \end{pmatrix}. \quad (1.244)$$

Consequently

$$u_{\lambda}(P) = \sqrt{E+m} \begin{pmatrix} \chi_{\lambda} \\ \frac{q\sigma^{3}}{E+m} \chi_{\lambda} \end{pmatrix}, \qquad (1.245)$$

which coincides with our former result (1.179).

# 1.9 Spin Sums and Projection Operators

Let us recall that negative energy solution were plane-waves of the form

$$v_{\lambda}(p)e^{ipx} = v_{\lambda}e^{i\omega_{p}t - i\boldsymbol{p}\cdot\boldsymbol{x}}, \qquad (1.246)$$

with amplitude v(p) satisfying

$$(\gamma^{\mu}p_{\mu} + m)v(p) = 0 \implies v(p) = \sqrt{E+m} \begin{pmatrix} \sigma \cdot p \\ E+m \chi \lambda \\ \chi \lambda \end{pmatrix}.$$
 (1.247)

We will now show that the following "ortho-normality" relations hold

$$\overline{u}_{\lambda}(p)u_{\lambda'}(p) = 2m\delta_{\lambda\lambda'},$$

$$\overline{v}_{\lambda}(p)v_{\lambda'}(p) = -2m\delta_{\lambda\lambda'},$$

$$\overline{u}_{\lambda}(p)v_{\lambda'}(p) = 0,$$

$$\overline{v}_{\lambda}(p)u_{\lambda'}(p) = 0,$$
(1.248)

where  $\overline{u}_{\lambda}(p) = u_{\lambda}^{\dagger}(p)\gamma^{0}$ ,  $\overline{v}_{\lambda}(p) = v_{\lambda}^{\dagger}(p)\gamma^{0}$ .

We already know that  $\overline{\psi}(x)\psi(x)$  is a Lorentz scalar, it is not difficult to see that also  $\overline{u}_{\lambda}(p)u_{\lambda'}(p)$ ,  $\overline{v}_{\lambda}(p)v_{\lambda'}(p)$ , and  $\overline{u}_{\lambda}(p)v_{\lambda'}(p)$  are Lorentz scalars. In fact, e.g.

$$\overline{u}_{L,\lambda}(p)v_{L,\lambda}(p) = \overline{u}_{\lambda}(L^{-1}p)S^{-1}(L)S(L)v_{\lambda}(L^{-1}p)$$
$$= \overline{u}_{\lambda}(L^{-1}p)v_{\lambda}(L^{-1}p). \qquad (1.249)$$

So, in order to prove (1.248) we can go to the rest frame where bisponors

acquire the simple form (cf. Eq. (1.182))

$$u_{1/2}(m, \mathbf{0}) = \sqrt{2m} \begin{pmatrix} 1\\0\\0\\0 \end{pmatrix}, \quad u_{-1/2}(m, \mathbf{0}) = \sqrt{2m} \begin{pmatrix} 0\\1\\0\\0 \end{pmatrix},$$
$$v_{1/2}(m, \mathbf{0}) = \sqrt{2m} \begin{pmatrix} 0\\0\\1\\0 \end{pmatrix}, \quad v_{-1/2}(m, \mathbf{0}) = \sqrt{2m} \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix}. \quad (1.250)$$

From these results (1.248) follow automatically.

Upshot of (1.248) is that the four bispinors  $u_{\lambda}(p)$  and  $v_{\lambda}(p)$  are linearly independent and so they form a complete basis in the space of Dirac spinors.

#### **Positive Definite Norm**

Normalization in (1.248) is Lorentz invariant, however, the *norm* is *not positive-definite*. In fact, we know that the positive-definite density per unit volume is

$$\rho(p) = J^0(p) = \bar{\psi}_p(x)\gamma^0\psi_p(x).$$

This indicates that instead of (1.248) one could use scalar product with  $\gamma^0$  insertion. This would indeed do, e.g.

$$\begin{split} \bar{\psi}_{\lambda,p}^{(+)}(x)\gamma^{0}\psi_{\lambda',p}^{(+)}(x) &= \bar{u}_{\lambda}(p)\gamma^{0}u_{\lambda'}(p) \\ &= \frac{1}{2m} \left[ \bar{u}_{\lambda}(p)\gamma^{0}p u_{\lambda'}(p) + \bar{u}_{\lambda}(p)p\gamma^{0}u_{\lambda'}(p) \right] \\ &= \frac{1}{2m} \bar{u}_{\lambda}(p)\{\gamma^{0},p\}u_{\lambda'}(p) = \frac{p^{0}}{m} \delta_{\lambda\lambda'} \,. \end{split}$$

Similarly, we can show that

$$\bar{v}_{\lambda}(p)\gamma^{0}v_{\lambda'}(p) = \frac{p^{0}}{m}\delta_{\lambda\lambda'}$$
 and  $\bar{v}_{\lambda}(\tilde{p})\gamma^{0}v_{\lambda'}(p) = 0$ ,

with  $\tilde{p}^{\mu} = (p^0, -p)$ . In deriving these relations we used that

$$\begin{split} \bar{u}_{\lambda}(p)(\not\!p-m) &= 0 &\Leftrightarrow \quad \frac{1}{m}\bar{u}_{\lambda}(p)\not\!p \,=\, \bar{u}_{\lambda}(p)\,,\\ \delta v_{\lambda}(p)(\not\!p+m) &= 0 \quad\Leftrightarrow \quad -\frac{1}{m}\bar{v}_{\lambda}(p)\not\!p \,=\, \bar{v}_{\lambda}(p)\,. \end{split}$$

For purpose of this section, however, the "scalar product" defined via (1.248) will suffice because *a*) it is simpler and *b*) the semidefiniteness of the norm will not play any conceptual role in our reasonings. To proceed, we observe that the following relations hold

$$\begin{aligned} (p - m)u_{\lambda}(p) &= 0, \\ (p + m)v_{\lambda}(p) &= 0, \\ (p - m)v_{\lambda}(p) &= (p + m - 2m)v_{\lambda}(p) = -2mv_{\lambda}(p), \\ (p + m)v_{\lambda}(p) &= (p - m + 2m)u_{\lambda}(p) = 2mu_{\lambda}(p). \end{aligned}$$
 (1.251)

Let us now consider the operators

$$\tilde{\Lambda}^{+}(p) = \sum_{\lambda} u_{\lambda}(p) \overline{u}_{\lambda}(p),$$
  

$$\tilde{\Lambda}^{-}(p) = \sum_{\lambda} v_{\lambda}(p) \overline{v}_{\lambda}(p).$$
(1.252)

When applied to positive and negative-energy bisponors they yield

$$\tilde{\Lambda}^{+}(p)u_{\lambda}(p) = \sum_{\lambda'} u_{\lambda'}(p)\overline{u}_{\lambda'}(p)u_{\lambda}(p) = 2m \sum_{\lambda'} u_{\lambda'}(p)\delta_{\lambda\lambda'} = 2mu_{\lambda}(p),$$
  
$$\tilde{\Lambda}^{+}(p)v_{\lambda}(p) = \sum_{\lambda'} u_{\lambda'}(p)\underbrace{\overline{u}_{\lambda'}(p)v_{\lambda}(p)}_{0} = 0.$$
 (1.253)

Similarly

$$\tilde{\Lambda}^{-}(p)u_{\lambda}(p) = 0$$
, and  $\tilde{\Lambda}^{-}(p)v_{\lambda}(p) = -2mv_{\lambda}(p)$ . (1.254)

By comparing these relations with operators  $(\gamma^{\mu}p_{\mu} \pm m)$  we can make the following identification:

$$\tilde{\Lambda}^{+}(p) = \sum_{\lambda'} u_{\lambda'}(p) \overline{u}_{\lambda'}(p) = \gamma^{\mu} p_{\mu} + m,$$
  

$$\tilde{\Lambda}^{-}(p) = \sum_{\lambda} v_{\lambda}(p) \overline{v}_{\lambda}(p) = \gamma^{\mu} p_{\mu} - m.$$
(1.255)

Let us now define two new operators

$$\Lambda^{+}(p) \equiv \frac{\tilde{\Lambda}^{+}(p)}{2m} = \frac{\gamma^{\mu}p_{\mu} + m}{2m},$$
  

$$\Lambda^{-}(p) \equiv -\frac{\tilde{\Lambda}^{-}(p)}{2m} = \frac{-(\gamma^{\mu}p_{\mu} - m)}{2m}.$$
(1.256)

It can be easily recognized that these operators are projection operators as they fulfill the necessary conditions for projection operators, in particular:

$$\left[ \Lambda^{\pm}(p) \right]^{2} = \left[ \frac{\pm (\gamma^{\mu} p_{\mu} \pm m)}{2m} \right]^{2} = \frac{(\gamma^{\mu} p_{\mu})^{2} \pm 2\gamma^{\mu} p_{\mu} m + m^{2}}{4m^{2}} \\ = \frac{\pm (\gamma^{\mu} p_{\mu} \pm m)}{2m} = \Lambda^{\pm}(p),$$

Let us also note that

$$\operatorname{Fr} \left( \Lambda^{\pm}(p) \right) = \frac{\pm \operatorname{Tr}(\gamma^{\mu} p_{\mu})}{2m} + 2$$
$$= \frac{\pm p_{\mu} \operatorname{Tr} \gamma^{\mu}}{2m} + 2 = 2. \qquad (1.257)$$

Projection operators  $\Lambda^+$  and  $\Lambda^-$  project over positive and negative energy states, respectively.

## 1.10 Electromagnetic Coupling of Electrons

#### Non-relativistic Charged Particle

For a free particle of mass *m*, the Hamiltonian is simply  $H_0 = p^2/2m$ . If the particle has charge *q*, then in the presence of an external electromagnetic field the Hamiltonian changes to

$$H = \frac{\left(p - \frac{q}{c}A\right)^2}{2m} + q\phi, \qquad (1.258)$$

where *A* and  $\phi$  are the vector and scalar potential, respectively.

Moreover, we also have to insist on a gauge condition which can be taken in the form  $\nabla \cdot A = 0$  (so-called Coulomb gauge). The magnetic field is connected with the vector potential via  $\boldsymbol{B} = \nabla \times A$  while scalar potential with electric field via  $\boldsymbol{E} = -\nabla \phi - \frac{\partial A}{\partial t}$ . So, in particular, situation with zero electric field and constant magnetic field  $\boldsymbol{B} = (0, 0, B)$  we can set  $\boldsymbol{A} = \frac{1}{2}B(-y, x, 0)$  and  $\phi = 0$ .

In this case we can write the Hamiltonian (1.258) to the first order in q as

$$H = \frac{1}{2m} \left[ p^2 - \frac{q}{c} (pA + Ap) \right] + O(q^2).$$
 (1.259)

In quantum mechanics,  $pA \neq Ap$ , but we can relate these two expressions via  $p^iA^i = A^ip^i + [p^i, A^i]$ , where  $[p^i, A^i] = -i\hbar [\nabla_i, A^i] = -i\hbar \nabla \cdot A = 0$  (in Coulomb gauge). Then

$$H = \frac{\boldsymbol{p}^2}{2m} - \frac{q}{mc}\boldsymbol{A}\cdot\boldsymbol{p} + O(q^2). \qquad (1.260)$$

By evaluating explicitly  $A \cdot p$  we get

$$A \cdot p = \frac{1}{2}B(-y, x, 0)(p_x, p_y, p_z) = \frac{B}{2}(xp_y - yp_x) = \frac{B}{2}L_z.$$
 (1.261)

Here  $L_z$  is 3rd component of the (orbital) angular momenta. Due to rotational invariance of the experimental setup we can easily generalize this result to arbitrarily oriented *B*. In particular, we can write  $A \cdot p = L \cdot B/2$ . Consequently, we get that the Hamiltonian (1.260) is composed of two parts  $H = H_0 + H_{\text{EM}}$ , where

$$H_{\rm EM} = -\frac{q}{2mc} \boldsymbol{B} \cdot \boldsymbol{L} \,. \tag{1.262}$$

The change from p to  $p - \frac{q}{c}A$  is known as *minimal substitution* and the ensuing interaction term is known as *minimal coupling*.

Generally, the commutator of a function f with the derivation  $\left[\frac{d}{dx}, f\right]$  is equal to  $\frac{df}{dx}$  since (operating on a test function u)

$$\left[\frac{d}{dx}, f\right] u = \left(\frac{d}{dx}(fu)\right) - f\frac{du}{dx} =$$
$$= \left(\frac{df}{dx}\right) u + f\frac{du}{dx} - f\frac{du}{dx} = \left(\frac{df}{dx}\right) u.$$

Particularly for electron it is conventional to write this in the form  $(q = e \text{ and } m = m_e)$ 

$$H_{\rm EM} = -\frac{e\hbar}{2m_ec}\frac{L}{\hbar} \cdot \boldsymbol{B} = -g_L \mu_{\rm B} \frac{L}{\hbar} \cdot \boldsymbol{B} = \boldsymbol{\mu} \cdot \boldsymbol{B}, \qquad (1.263)$$

where  $\mu_{\rm B} = e\hbar/(2m_ec)$  is the *Bohr magneton*. The factor  $g_L$  is known a the *g*-factor (here  $g_L = 1$ ) and  $\mu$  the *orbital magnetic moment* of an electron. The term  $g_L \mu_{\rm B}$  is known as the *gyromagnetic ratio*.

Experimental atomic physics tells us that:

- ▶ electrons have spin 1/2
- ▶ gyromagnetic ratio for spin 1/2 particle is twice the gyromagnetic ratio for orbital angular momentum (i.e.  $g_s = 2g_L$ ).

The great achievement of Dirac was to show that his equation allows to consistently handle quantum theory of electron and to incorporate both aforementioned experimental observations. We will also see that Dirac's equation can do even more, namely it ensures that to each 1/2particle must exists *antiparticle* and it correctly predicts *fine structure* in the spectrum of hydrogen atom.

#### Minimal Electromagnetic Coupling and Dirac Equation

Let us now derive the gyromagnetic ratio for spin 1/2 particle directly from Dirac's equation.

When considering a relativistic situation, we have to work with the four-potential  $A_{\mu}$ . The minimal coupling prescription is then given by

$$p_{\mu} \rightarrow p_{\mu} - qA_{\mu} \Rightarrow \partial_{\mu} \rightarrow \partial_{\mu} + iqA_{\mu},$$
 (1.264)

where  $p_{\mu} = i \frac{\partial}{\partial x^{\mu}}$ , respectively. It is easy to see that the space components of this prescription provide consistent minimal prescription known from non-relativistic physics, namely

$$p_i \rightarrow p_i - qA_i \Leftrightarrow p^i \rightarrow p^i - qA^i \Leftrightarrow -i\nabla \rightarrow -i\nabla - qA$$
. (1.265)

With this notation the Dirac equation takes the form

$$(i\partial - qA - m)\psi(x) = 0.$$
(1.266)

This can be further rewritten in the Schrödinger-like form

$$i\frac{\partial\psi}{\partial t} = [\alpha(-i\nabla - qA) + \beta m + q\phi]\psi$$
  
=  $[\alpha p + \beta m]\psi + [-q\alpha A + q\phi]\psi$   
=  $(H_0 + H_{int})\psi$ . (1.267)

To extract more physics, let us concentrate on the non-relativistic limit.

We write  $\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix}$  and use Dirac's representation. Then from

$$i\frac{\partial\psi}{\partial t} = \begin{bmatrix} \begin{pmatrix} 0 & \sigma \\ \sigma & 0 \end{pmatrix} (-i\nabla - q\mathbf{A}) + \begin{pmatrix} q\phi + m & 0 \\ 0 & q\phi - m \end{pmatrix} \end{bmatrix} \psi, \quad (1.268)$$

we get two coupled equations

$$i\frac{\partial\varphi}{\partial t} = \boldsymbol{\sigma} \cdot \boldsymbol{\Pi}\chi + q\phi\varphi + m\varphi,$$
  

$$i\frac{\partial\chi}{\partial t} = \boldsymbol{\sigma} \cdot \boldsymbol{\Pi}\varphi + q\phi\chi - m\chi. \qquad (1.269)$$

Here we have introduced the so-called *kinetic momentum*  $\hat{\Pi}_{\mu}$  as

$$p_{\mu} - qA_{\mu} = \Pi_{\mu} \quad \Rightarrow \quad -i\nabla - qA = \Pi . \tag{1.270}$$

Similarly as for a free particle we pass to the non-relativistic limit by factoring out from  $\psi$  the fast oscillating factor, i.e.

$$\psi = \begin{pmatrix} \varphi \\ \chi \end{pmatrix} = e^{-imt} \begin{pmatrix} \tilde{\varphi} \\ \tilde{\chi} \end{pmatrix}.$$
(1.271)

With this Eq. (1.269) reduces to

$$i\frac{\partial\tilde{\varphi}}{\partial t} = \sigma \cdot \Pi\tilde{\chi} + q\phi\tilde{\varphi}, \qquad (1.272)$$

$$i\frac{\partial\tilde{\chi}}{\partial t} = \boldsymbol{\sigma}\cdot\boldsymbol{\Pi}\tilde{\varphi} + q\phi\tilde{\chi} - 2m\tilde{\chi}. \qquad (1.273)$$

Since in Eq. (1.273) the  $2m\tilde{\chi}$  term dominates over  $i\partial\tilde{\chi}/\partial t$  we can drop the  $i\partial\tilde{\chi}/\partial t$  term and rewrite Eq. (1.273) as

$$\tilde{\chi} = \frac{\sigma \Pi}{2m} \tilde{\varphi} + \frac{q\phi}{2m} \tilde{\chi} \sim \frac{\sigma \Pi}{2m} \tilde{\varphi}, \qquad (1.274)$$

where the last approximation reflects the fact that the interaction energy  $q\phi$  is typically much smaller than the rest-mass energy  $mc^2$ , so  $|q\phi/2mc^2| \ll 1$ .

Inserting Eq. (1.274) into Eq. (1.272), we get

$$i\frac{\partial\tilde{\varphi}}{\partial t} = \left(\frac{(\boldsymbol{\sigma}\cdot\boldsymbol{\Pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\Pi})}{2m}\right)\tilde{\varphi} + q\phi\tilde{\varphi} = \left(\frac{(\boldsymbol{\sigma}\cdot\boldsymbol{\Pi})(\boldsymbol{\sigma}\cdot\boldsymbol{\Pi})}{2m} + q\phi\right)\tilde{\varphi}.$$
 (1.275)

This can further be reduced by using an analogue of the well known identity

$$(\boldsymbol{\sigma} \cdot \boldsymbol{a})(\boldsymbol{\sigma} \cdot \boldsymbol{b}) = \sigma^{i} \sigma^{j} a^{i} b^{j} = (\delta^{ij} + i \varepsilon^{ijk} \sigma^{k}) a^{i} b^{j}$$
$$= \boldsymbol{a} \cdot \boldsymbol{b} + i \sigma^{k} (\boldsymbol{a} \times \boldsymbol{b})^{k}$$
$$= \boldsymbol{a} \cdot \boldsymbol{b} + i \boldsymbol{\sigma} \cdot (\boldsymbol{a} \times \boldsymbol{b}), \qquad (1.276)$$

which is true only if *a* and *b* are c-numbered vectors. For operators, this identity must be modified. In particular, if *a* and *b* are generic

vector operators we should write

$$(\boldsymbol{\sigma} \cdot \boldsymbol{a})(\boldsymbol{\sigma} \cdot \boldsymbol{b}) = \frac{1}{4} \left\{ \sigma^{i}, \sigma^{j} \right\} \left\{ a^{i}, b^{j} \right\} + \frac{1}{4} \left[ \sigma^{i}, \sigma^{j} \right] \left[ a^{i}, b^{j} \right], \quad (1.277)$$

where we used the decomposition into a symmetric and an antisymmetric parts. Specifically, for the scalar products of  $\sigma$  with the kinetic momentum, we get

$$(\boldsymbol{\sigma} \cdot \boldsymbol{\Pi})(\boldsymbol{\sigma} \cdot \boldsymbol{\Pi}) = \frac{1}{4} 2\delta^{ij} \left\{ \Pi^{i}, \Pi^{j} \right\} + \frac{1}{4} 2i\varepsilon^{ijk} \sigma^{k} \left[ \Pi^{i}, \Pi^{j} \right]$$
$$= \boldsymbol{\Pi}^{2} + \frac{1}{2}i\varepsilon^{ijk} \sigma^{k} \left[ p^{i} - qA^{i}, p^{j} - qA^{j} \right]$$
$$= \boldsymbol{\Pi}^{2} - \frac{1}{2}i\varepsilon^{ijk} \sigma^{k} q \left( \left[ p^{i}, A^{j} \right] + \left[ A^{i}, p^{j} \right] \right)$$
$$= \boldsymbol{\Pi}^{2} - \frac{1}{2}q\sigma^{k}\varepsilon^{ijk} \left( \nabla_{i}A^{j} - \nabla_{j}A^{i} \right)$$
$$= \boldsymbol{\Pi}^{2} - q\sigma^{k} (\nabla \times A)^{k} = \boldsymbol{\Pi}^{2} - q\boldsymbol{\sigma} \cdot \boldsymbol{B}. \quad (1.278)$$

Thus, Eq. (1.275) finally reduces to

$$i\frac{\partial\tilde{\varphi}}{\partial t} = \left[\frac{(\boldsymbol{p}-q\boldsymbol{A})^2}{2m} - \frac{q\boldsymbol{\sigma}\cdot\boldsymbol{B}}{2m} + q\boldsymbol{\phi}\right]\tilde{\varphi}, \qquad (1.279)$$

which is nothing but the Pauli equation of the non-relativistic quantum physics. Hence we gain certain confidence that we are on the right track.

We can again write the Dirac Hamiltonian in (1.279) as  $H_0 + H_{\text{EM}}$ . By restoring  $\hbar$  and c we get

$$H_{\rm EM} = -\frac{e\hbar}{2mc}\frac{L}{\hbar} \cdot \boldsymbol{B} - \frac{q\hbar}{2mc}\frac{\boldsymbol{\sigma}}{\hbar} \cdot \boldsymbol{B}$$
$$= -\frac{e\hbar}{2mc}\frac{L}{\hbar} \cdot \boldsymbol{B} - \frac{q\hbar}{mc}\frac{\hat{\boldsymbol{\sigma}}}{\hbar} \cdot \boldsymbol{B}, \qquad (1.280)$$

where  $\hat{\sigma} = \sigma/2$  is generator of rotations for spin-1/2 particles. Specifically for electrons we can write

$$H_{\rm EM} = -g_L \mu_{\rm B} \frac{L}{\hbar} \cdot \boldsymbol{B} - g_s \mu_{\rm B} \frac{\hat{\boldsymbol{\sigma}}}{\hbar} \cdot \boldsymbol{B}$$
$$= \mu \cdot \boldsymbol{B}, \qquad (1.281)$$

where

$$\mu = -\mu_{\rm B} \left( g_L L + g_s \hat{\sigma} \right) \,, \tag{1.282}$$

is the total magnetic moment. Note that  $g_s = 2g_L = 2$ . The fact that  $g_s = 2$  is a nontrivial prediction of Dirac theory derived within the non-relativistic context of the Dirac equation. The *g*-factor of electron has now been measured to something like 12 figures of accuracy and it is not precisely 2, it differs by a tiny amount. Understanding this small difference goes, however, beyond Dirac's theory as it requires a full-fledged Quantum Field Theory.

Recall that  $(\nabla \times A)^k = \varepsilon^{klm} \partial_l A^m$ , i.e.  $2(\nabla \times A)^k = \varepsilon^{klm} (\partial_l A^m - \partial_m A^l).$ 

The current value of electron *g*-factor is give by  $g_s/2 = 1,001159652180...$ 

## 1.11 Representations of Gamma Matrices

We have seen that  $\gamma$ -matrices satisfy the defining relation

$$\{\gamma^{\mu}, \gamma^{\nu}\} = 2\eta^{\mu\nu}.$$
 (1.283)

The question naturally arises, how uniquely are the  $\gamma$ -matrices determined by the Clifford product (1.283). This is answered by the so-called *Fundamental theorem of Clifford algebra* (W. Pauli 1936):

**Theorem 1.11.1** (Fundamental theorem of Clifford algebra) If two distinct sets of  $\gamma$ -matrices are given, that both satisfy the Clifford algebra relation

 $\{\gamma^{\mu},\gamma^{\nu}\} = 2\eta^{\mu\nu},$ 

then they are connected to each other by similarity transformation

$$\gamma^{\prime\mu} = S^{-1}\gamma^{\mu}S$$

If, in addition, the  $\gamma$ -matrices are (anti-)Hermitian (as in Dirac's particular case where  $\gamma^0 = \gamma^{0\dagger}$  and  $\gamma^i = -\gamma^{i\dagger}$ ) then **S** itself is unitary, i.e.

$$\gamma^{\prime \mu} = U^{\dagger} \gamma^{\mu} U.$$

This transformation is unique up to a multiplicative factor, which in case of U must have absolute value 1.

Though all physical consequences should be independent of a particular choice of  $\gamma$ -matrics representation, different sets might present different technical advantages.

Let us now review the most typical representations of  $\gamma$ -matrices.

#### **Dirac's Representation**

So far we worked with the so-called Dirac's representation of  $\gamma$ -matrices. This is historically the oldest representation of  $\gamma$ -matrices. It was found by Dirac — hence the name *Dirac's representation*. In this representation  $\gamma$  matrices are given by

$$\gamma^{0} = \begin{pmatrix} \mathbb{1} & 0\\ 0 & -\mathbb{1} \end{pmatrix}, \quad \gamma^{i} = \begin{pmatrix} 0 & \sigma_{i}\\ -\sigma_{i} & 0 \end{pmatrix}, \quad \gamma^{5} = \begin{pmatrix} 0 & \mathbb{1}\\ \mathbb{1} & 0 \end{pmatrix}.$$
(1.284)

By using properties of tensor product, we can conveniently rewrite these matrices as

$$\gamma^0 = \sigma_3 \otimes \mathbb{1}, \quad \gamma = i\sigma_2 \otimes \sigma, \quad \gamma^5 = \sigma_1 \otimes \mathbb{1}.$$
 (1.285)

This representation is particularly convenient for taking the non-relativistic limit, e.g., for a free particle we have already seen that in Dirac's representation

$$\begin{pmatrix} \chi \\ \frac{\boldsymbol{\sigma} \cdot \boldsymbol{p}}{E+m} \chi \end{pmatrix} \xrightarrow{\text{NR}} \begin{pmatrix} \chi_{NR} \\ 0 \end{pmatrix}.$$
(1.286)

Clearly when a set of  $\gamma^{\mu}$  matrices satisfies Clifford algebra product (1.283) and is (anti)Hermitian, then also  $\gamma'^{\mu} = U^{\dagger}\gamma^{\mu}U$  satisfy the Clifford product and are (anti)Hermitian. Hard part of the proof of Theorem 1.11.1 is to show existence and uniqueness of U.

An analogous behavior was also observed for Dirac's wave function of an electron in external electromagnetic field.

Let us also recall that the Lorentz group elements associated with rotations and boosts have in Dirac's representation the explicit forms (cf. Eq. (1.215) and Eq. (1.241))

$$S_D(\mathbf{R}) = \begin{pmatrix} e^{-\frac{i}{2}\mathbf{n}_k\sigma_k} & 0\\ 0 & e^{-\frac{i}{2}\mathbf{n}_k\sigma_k} \end{pmatrix}, \qquad (1.287)$$

$$S_D(\boldsymbol{B}) = \sqrt{\frac{E+m}{2m}} \begin{pmatrix} \mathbf{1} & \frac{\boldsymbol{p}\cdot\boldsymbol{\sigma}}{E+m} \\ \frac{\boldsymbol{p}\cdot\boldsymbol{\sigma}}{E+m} & \mathbf{1} \end{pmatrix}.$$
(1.288)

#### **Chiral (Weyl) Representation**

Another important representation is *chiral or Weyl representation* that is given by

$$\gamma^{0} = \begin{pmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{pmatrix}, \quad \gamma^{i} = \begin{pmatrix} 0 & \sigma_{i} \\ -\sigma_{i} & 0 \end{pmatrix}, \quad \gamma^{5} = \begin{pmatrix} -\mathbb{1} & 0 \\ 0 & \mathbb{1} \end{pmatrix}.$$
(1.289)

And again, we can rewrite this representation in terms of tensor products as

$$\gamma^0 = \sigma_1 \otimes \mathbb{1}, \quad \gamma = i\sigma_2 \otimes \sigma, \quad \gamma^5 = \sigma_3 \otimes \mathbb{1}.$$
 (1.290)

This representation is important for description of massless spin 1/2 particles as in this representation the Dirac massless equation decouples into two autonomous equations, one for upper and one for the lower component of the Dirac spinor.

Chiral representation is also instrumental in discussions related to bispinor representation of Lorentz group. To this end we recall that for rotations we can write

$$S(\mathbf{R}) = e^{-\frac{i}{4}\omega_{ij}\sigma^{ij}}, \quad i, j = 1, 2, 3, \qquad (1.291)$$

with  $\sigma^{ij} = \frac{i}{2}[\gamma^i, \gamma^j] = i\gamma^i\gamma^j$ . By defining

$$\sigma^{ij} = 2\varepsilon^{ijk}\hat{\sigma}^k = 2\varepsilon^{ijk} \begin{pmatrix} \frac{\sigma_k}{2} & 0\\ 0 & \frac{\sigma_k}{2} \end{pmatrix}, \qquad (1.292)$$

we get

$$S_W(\mathbf{R}) = e^{-i\boldsymbol{\theta}\cdot\hat{\boldsymbol{\sigma}}} = \begin{pmatrix} e^{-\frac{i}{2}\boldsymbol{\theta}\cdot\boldsymbol{\sigma}} & 0\\ 0 & e^{\frac{i}{2}\boldsymbol{\theta}\cdot\boldsymbol{\sigma}} \end{pmatrix}.$$
 (1.293)

This has clearly the same structure both in chiral and Dirac's representation because  $\gamma^i$ , i = 1, 2, 3 are the same.

On the other hand, general boost in bispinor representation is given by the prescription

$$S(\mathbf{B}) = e^{-\frac{i}{2}\omega_{0i}\sigma^{0i}} = e^{\frac{1}{2}\zeta_{i}\gamma^{0}\gamma^{i}}.$$
 (1.294)

By using the fact that in the chiral representation

$$\boldsymbol{\sigma}^{0i} = i \begin{pmatrix} -\boldsymbol{\sigma} & 0\\ 0 & \boldsymbol{\sigma} \end{pmatrix}, \qquad (1.295)$$

we get that

$$S_W(\boldsymbol{B}) = e^{\frac{\boldsymbol{\zeta} \cdot \boldsymbol{\gamma}^0 \boldsymbol{\gamma}}{2}} = \begin{pmatrix} e^{-\frac{\boldsymbol{\zeta} \cdot \boldsymbol{\sigma}}{2}} & 0\\ 0 & e^{\frac{\boldsymbol{\zeta} \cdot \boldsymbol{\sigma}}{2}} \end{pmatrix}.$$
(1.296)

Since the group elements  $S_W(\mathbf{R})$  and  $S_W(\mathbf{B})$  have a block diagonal form it seems that the bispinor representation is *reducible* to two independent spinor representations. So apparently we do not need to work with bispinors, but it would be enough to work with spinors only. This, indeed, is true for massless particles. For massive particles the issue is more complicated and is related to the concept of *parity*.

In order to understand this better we should discuss discrete transformations of Lorentz group. This will be done in the following section.

## 1.12 Discrete transformations

### **Space Reflection (Parity) Transformation**

Parity transformation is acting on the position 4-vector as follows:

$$x^{\mu} = (t, \mathbf{x}) \xrightarrow{P} x^{\mu}_{P} = (t, -\mathbf{x}).$$
 (1.297)

From this we can see, that this transformation can be written in the form

$$x_P^{\mu} = \mathbf{P}^{\mu}{}_{\nu} x^{\nu} , \qquad (1.298)$$

where the matrix **P** reads

$$\boldsymbol{P}^{\mu}{}_{\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} = \eta^{\mu\nu} = \eta_{\mu\nu}.$$
(1.299)

This satisfies the defining property of Lorentz group, namely

$$\boldsymbol{P}_{\alpha}^{\ \mu}\eta_{\mu\nu}\boldsymbol{P}^{\nu}{}_{\beta} = \eta_{\alpha\beta}, \qquad (1.300)$$

and hence *P* is an element of Lorentz group. We can also see that det P = -1, so it corresponds to an improper orthochronous Lorentz transformation.

To find the bispinor representation of the parity transformation, we recall that the covariance of Dirac equation under Lorentz group requires that (cf. Eq. (1.107))

$$S(\boldsymbol{P})\gamma^{\mu}S^{-1}(\boldsymbol{P}) = \boldsymbol{P}_{\nu}^{\ \mu}\gamma^{\nu} \quad \Leftrightarrow \quad S^{-1}(\boldsymbol{P})\gamma^{\mu}S(\boldsymbol{P}) = \boldsymbol{P}^{\mu}_{\ \nu}\gamma^{\nu}, \quad (1.301)$$

should be satisfies. In this case, we cannot solve the equation in terms of infinitesimal transformations. Fortunately, it can be solved directly. In this case note that

Note that  $\delta_{\mu 0}$  and  $\gamma^{\mu}$  are not Einstein summed.

$$S(\mathbf{P}) \gamma^{\mu} S^{-1}(\mathbf{P}) = -(-1)^{\delta_{\mu 0}} \gamma^{\mu}. \qquad (1.302)$$

Using the fact, that  $\{\gamma^0, \gamma^\mu\} = 2\eta^{0\mu}$ , we obtain that

$$\gamma^{0}\gamma^{\mu} = -\gamma^{\mu}\gamma^{0} + 2\eta^{0\mu}$$
  
= 
$$\begin{cases} -1 + 2 \cdot 1 = 1, \ \mu; & \text{for } \mu = 0 \\ -\gamma^{i}\gamma^{0}; & \text{for } \mu \neq 0, \ \mu = i. \end{cases}$$
 (1.303)

Take  $S(\mathbf{P}) = \gamma^0$ , then (1.302) reduces to the

$$\gamma^{0}\gamma^{\mu}(\gamma^{0})^{-1} = \gamma^{0}\gamma^{\mu}\gamma^{0} = -(-1)^{\delta_{\mu 0}}\gamma^{\mu}.$$
(1.304)

Most generally, we can chose  $S(\mathbf{P})$  to be

$$S(\boldsymbol{P}) = e^{i\phi}\gamma^0. \tag{1.305}$$

So, finally the parity transformed bispinor takes the form

$$\psi_P(x) = S(\mathbf{P})\psi(\mathbf{P}^{-1}x) = e^{i\phi}\gamma^0\psi(\mathbf{P}^{-1}x) = e^{i\phi}\gamma^0\psi(x_P). \quad (1.306)$$

If one requires that after two parity transformations one should return to the original state, i.e.,  $S(\mathbf{P})\psi_P(x_P) = \psi(x)$  then

$$e^{i2\phi}(\gamma^0)^2\psi(x) = e^{i2\phi}\psi(x) = \psi(x).$$
(1.307)

This implies that  $\phi = 0$  or  $\phi = \pi$  (modulo  $2\pi$ ) or, in other words, that

$$S(\boldsymbol{P}) = \pm \gamma^0 = \eta_P \gamma^0, \qquad (1.308)$$

where  $\eta_P$  is the so-called *intrinsic parity*, i.e, yet another quantum number of a particle. Result (1.308) is, however, not entire correct. In fact, let us consider a bispinor representation of rotations, i.e.

$$\psi_{\boldsymbol{R}}(x) = S(\boldsymbol{R})\psi(\boldsymbol{R}^{-1}x) = \begin{pmatrix} e^{-\frac{i}{2}\boldsymbol{\theta}\cdot\boldsymbol{\sigma}} & 0\\ 0 & e^{-\frac{i}{2}\boldsymbol{\theta}\cdot\boldsymbol{\sigma}} \end{pmatrix}\psi(\boldsymbol{R}^{-1}x). \quad (1.309)$$

For  $2\pi$  rotation around *z*-axis we get:

$$S(\mathbf{R}, \theta = 2\pi, \text{around } z\text{-axis})\psi(x) = \begin{pmatrix} e^{-i\pi\sigma_3} & 0\\ 0 & e^{-i\pi\sigma_3} \end{pmatrix}\psi(x)$$
$$= \begin{pmatrix} -\mathbb{1} & 0\\ 0 & -\mathbb{1} \end{pmatrix}\psi(x) \neq \begin{pmatrix} \mathbb{1} & 0\\ 0 & \mathbb{1} \end{pmatrix}\psi(x).$$
(1.310)

Hence, one should rotate by  $4\pi$  around *z* axis to get the original bispinor. Since  $4\pi$  rotation is an analogue of 4 reflections we should require that after 4 (and not 2) reflections the Dirac particle will get back to its original state  $\psi(x)$ . With this we finally get

$$S(\mathbf{P})\psi(x) = \pm i\gamma^{0}\psi(x) = i\eta_{P}\gamma^{0}\psi(x).$$
 (1.311)

Since in the Weyl representation

$$\gamma^{0} = \begin{pmatrix} 0 & \mathbb{1} \\ & & \\ mathbb1 & 0 \end{pmatrix}, \qquad (1.312)$$

we see that under parity transformation the upper and lower spinors are interchanged in the bispinor. Hence, if we wish to work with a parity invariant 1/2-spin fermion, we must describe it with a bispinor wave function and Dirac's equation is the equation that stipulates the corresponding dynamics.

As an example of application of a parity transformation we consider now the positive-energy Dirac wave function for a free particle with momentum *p*. Then

$$u(p,\lambda)e^{-ipx} \to \pm i\gamma^0 u(p,\lambda)e^{-ipx_P} = \pm iu(p_P,\lambda)e^{-ip_Px}.$$
(1.313)

Rewriting this in more detail and recalling that in the Dirac representation  $\gamma^0 = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}$  and  $u(p, \lambda) \propto \begin{pmatrix} \chi_\lambda \\ \underline{\sigma \cdot p} \\ E+m \chi_\lambda \end{pmatrix}$ :

$$\begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix} \begin{pmatrix} \chi_{\lambda} \\ \frac{\boldsymbol{\sigma} \cdot \boldsymbol{p}}{E+m} \chi_{\lambda} \end{pmatrix} = \begin{pmatrix} \chi_{\lambda} \\ \frac{-\boldsymbol{\sigma} \cdot \boldsymbol{p}}{E+m} \chi_{\lambda} \end{pmatrix} = \begin{pmatrix} \chi_{\lambda} \\ \frac{\boldsymbol{\sigma} \cdot \boldsymbol{p}_{P}}{E+m} \chi_{\lambda} \end{pmatrix}.$$
 (1.314)

Here we have introduced a paritity transformed 4-momenta

$$p_P^{\mu} = (p_0, -\boldsymbol{p}) = (p_0, \boldsymbol{p}_P).$$
 (1.315)

Note, in particular, that the spatial part of the momentum has been parity transformed in (1.313), but the spin state has been unaltered. This is precisely what we would expect from parity transformation.

Similarly, we can now proceed with negative-energy solutions. In particular

$$v(p,\lambda)e^{ipx} = \pm i\gamma^0 v(p,\lambda)e^{ipx_p} = \mp iv(p_p,\lambda)e^{ip_px}.$$
(1.316)

So, the positive and negative-energy solutions have relative opposite intrinsic parities. After the reinterpretation of negative energy solutions this will imply that intrinsic parities for particle and antiparticle are reversed.

#### Parity of a Scalar Particle

For a complex wave function  $\phi(x)$  of a relativistic scalar (Klein–Gordon) particle one can follow the usual prescription for Lorentz group transformation of scalar functions, i.e.

$$\phi(x) \to \phi_L(x) = \phi(L^{-1}x),$$
 (1.317)

which in the parity case are phrased as

$$\phi(x) \to \phi_P(x) = \eta_P \phi(x_P).$$

Reason why  $\eta_P$  appears at all is that prescription (1.317) is valid only for *restricted Lorentz group*, i.e., the set of all Lorentz transformations that can be connected to the identity element by a continuous curve lying in the group. Passage to some of the remaining 3 component of Lorentz group is accompanied by an appearance of intrinsic quantum numbers. Consistency of this prescription can be checked by looking at a state with a definite momentum  $\phi(p, x) = e^{-ipx}$ . In this case the prescription gives

$$\phi_P(p, x) = \{e^{-ipx_P}\} = e^{-ip_P x} = \phi(p_P, x).$$

### **Time Reversal**

Time reversal transformation acts on a position 4-vector so that

$$x^{\mu} \rightarrow x_{T}^{\mu} = (t, \mathbf{x})^{T} = (-t, \mathbf{x}).$$
 (1.318)

This transformation can be described via transformation matrix

$$\boldsymbol{T}^{\mu}_{\ \nu} = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = -\eta^{\mu\nu} = -\eta_{\mu\nu}, \quad (1.319)$$

which again satisfies the defining relation of Lorentz group

$$T_{\alpha}^{\ \mu}\eta_{\mu\nu}T^{\nu}{}_{\beta} = \eta_{\alpha\beta}. \qquad (1.320)$$

Again, we can see that  $T_{\alpha}^{\mu}$  is an element of a Lorentz group. Since det T = -1 and  $T_{0}^{0} = -1$ , this discrete group element corresponds to an improper non-orthochronous Lorentz transformation.

Let us also mention other important vector quantities, namely velocity, momentum and angular momentum and their respective time reversals

$$\mathbf{v} \xrightarrow{T} \mathbf{v}_T = -\mathbf{v}, \quad \mathbf{p} \xrightarrow{T} \mathbf{p}_T = -\mathbf{p}, \quad \mathbf{J} \xrightarrow{T} \mathbf{J}_T = -\mathbf{J}.$$
 (1.321)

To find a bispinor representation of time reversal we cannot follow the same route as we did in the case of parity. This is because time reversal must be implemented via anti-unitary transformation (i.e., complex conjugation of the wave function is required) and Eq. (1.107) was not derived under such an assumption.

In non-relativistic quantum mechanics we know that the complete effect of a linear operator can be determined by specifying its action on a basis set of the vector space of physical states and then extend its application by exploiting the linearity of the maps. Similarly, the complete effect of an antilinear map can be determined by specifying its effect on a basis and extending the results using its *antilinearity*. Take, for instance, the momentum basis  $|p\rangle$ . Then  $\hat{T} |p\rangle = |-p\rangle$ . A generic state would then look like

$$|\psi\rangle = \sum_{p} \widetilde{\psi}(p) |p\rangle$$
 (1.322)

From this we can see, that effect of time reversal is then

$$\hat{T} |\psi\rangle = \hat{T} \sum_{p} \widetilde{\psi}(p) |p\rangle = \sum_{p} \widetilde{\psi}^{*}(p) \hat{T} |p\rangle$$

$$= \sum_{p} \widetilde{\psi}^{*}(p) |-p\rangle = \sum_{p} \widetilde{\psi}^{*}(-p) |p\rangle$$

$$= \sum_{p} \widetilde{\psi}_{T}(p) |p\rangle = |\psi_{T}\rangle . \qquad (1.323)$$

Thus we have that  $\tilde{\psi}_T(p) = \tilde{\psi}^*(-p)$  for scalar wave functions. If the state  $|\phi\rangle = \sum_p \tilde{\phi}(p) |p\rangle$  is defined similarly, then the scalar product

$$\begin{aligned} \langle \phi | \psi \rangle &= \sum_{p} \widetilde{\phi}^{*}(p) \widetilde{\psi}(p) = \sum_{p} \widetilde{\phi}^{*}(-p) \widetilde{\psi}(-p) \\ &= \left[ \sum_{p} \widetilde{\phi}(-p) \widetilde{\psi}^{*}(-p) \right]^{*} = \left[ \sum_{p} \widetilde{\phi}_{T}(p) \widetilde{\psi}_{T}(p) \right]^{*} \\ &= \langle \phi_{T} | \psi_{T} \rangle^{*} . \end{aligned}$$
(1.324)

In order to get *x*-representation of our wave function we can apply Fourier transformation thus obtaining

$$\psi_{T}(\mathbf{x}) = \int \widetilde{\psi}_{T}(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{x}}d\mathbf{p} = \int \widetilde{\psi}^{*}(-\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{x}}d\mathbf{p}$$
$$= \int \widetilde{\psi}^{*}(\mathbf{p})e^{i\mathbf{p}\cdot\mathbf{x}}d\mathbf{p} = \left[\int \widetilde{\psi}(\mathbf{p})e^{-i\mathbf{p}\cdot\mathbf{x}}\right]^{*} = \psi^{*}(\mathbf{x}). \quad (1.325)$$

In line with non-relativistic quantum mechanics, the effect of time reversal on the Dirac wave function can be written in the form

$$\psi_T(x) = \mathbf{B}\psi^*(x_T), \qquad (1.326)$$

where the matrix **B** acts on bispinorial indices.

To find *B* we complex conjugate Dirac equation and observe that the following chain of equivalencies holds

$$\left(i\gamma^{\mu}\frac{\partial}{\partial x^{\mu}} - m\right)\psi(x) = 0$$

$$\Leftrightarrow \qquad \left(i\gamma^{\mu}\frac{\partial}{\partial x_{T}^{\mu}} - m\right)\psi(x_{T}) = 0$$

$$\Leftrightarrow \qquad \left(i\gamma^{0*}\partial_{t} - i\gamma^{i*}\partial_{i} - m\right)\psi^{*}(x_{T}) = 0. \quad (1.327)$$

If we assume that the matrix **B** is defined so that

$$\boldsymbol{B}\left(\boldsymbol{\gamma}^{0*},-\boldsymbol{\gamma}^{i*}\right)\boldsymbol{B}^{-1} = \left(\boldsymbol{\gamma}^{0},\boldsymbol{\gamma}^{i}\right), \qquad (1.328)$$

then with the definition of  $\psi_T(x)$  in (1.326) we get

$$0 = \boldsymbol{B} \left( i \gamma^{0*} \partial_t - i \gamma^{i*} \partial_i - m \right) \psi^*(x_T) = \left( i \gamma^{\mu} \partial_{\mu} - m \right) \psi_T(x) \,. \tag{1.329}$$

Since matrices  $(\gamma^{0*}, -\gamma^{i*})$  satisfy Clifford algebra, the similarity transformation (1.328) is guaranteed by the Fundamental theorem of Clifford algebra.

Note that from (1.325) also follows that  $\psi_T(\mathbf{x}, t) = \left[e^{-i\mathbf{H}t}\psi^*(\mathbf{x}, 0)\right]$ =  $\left[e^{i\mathbf{H}t}\psi(\mathbf{x}, 0)\right]^* = \psi^*(\mathbf{x}, -t) = \psi^*(\mathbf{x}_T)$ . This clearly shows that  $\psi_T(x)$  satisfies Dirac's equation if  $\psi(x)$  does. The Fundamental theorem of Clifford algebra ensures that (aside from a phase factor) *B* is unitary.

To retrieve B from (1.328) we will use the fact that

$$\begin{aligned} \gamma^{0\dagger} &= \gamma^0 \implies \gamma^{0*} = (\gamma^0)^t , \\ \gamma^{i\dagger} &= -\gamma^i \implies \gamma^{i*} = -(\gamma^i)^t , \end{aligned} \tag{1.330}$$

and

$$C(\gamma^{\mu})^{t}C^{-1} = -\gamma^{\mu}.$$
 (1.331)

Here  $C = i\gamma^0\gamma^2$  is a *charge conjugation matrix* (which will be derived in the following section). With this we can write *B* in the form

$$\boldsymbol{B} = \eta_T \gamma_5 \boldsymbol{C} = i\eta_T \gamma^0 \gamma^1 \gamma^2 \gamma^3 i \gamma^0 \gamma^2 = \eta_T \gamma^1 \gamma^3$$
$$= \eta_T \begin{pmatrix} 0 & \sigma^1 \\ -\sigma^1 & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma^3 \\ -\sigma^3 & 0 \end{pmatrix} = \eta_T \begin{pmatrix} i\sigma^2 & 0 \\ 0 & i\sigma^2 \end{pmatrix}. \quad (1.332)$$

Here  $\eta_T$  is a complex number of unit amplitude, that is allowed by the Fundamental theorem of Clifford algebra. It is easy to see that *B* proposed in (1.332) satisfies (1.328). Indeed

$$B(\gamma^{0})^{*}B^{-1} = \gamma_{5}C(\gamma^{0})^{t}C^{-1}\gamma_{5} = \gamma^{0},$$
  

$$B(\gamma^{i})^{*}B^{-1} = -\gamma_{5}C(\gamma^{i})^{t}C^{-1}\gamma_{5} = -\gamma^{i}.$$
 (1.333)

Note that since  $\gamma^1$  and  $\gamma^3$  are identical both in Dirac's and chiral representation, the form (1.332) remains the same in both representations. Consequently, time reversal (in contrast to parity) does not swap upper and lower components of Dirac's bispinor.

To find a constraint on the phase factor  $\eta_T$  we might require that  $(\psi_T)_T = \psi$ . This in turn gives

$$\psi(x) = [\psi_T(x)]_T = \eta_{TT} \gamma^1 \gamma^3 \left[ \eta_T \gamma^1 \gamma^3 \psi^*(x) \right]^* = -\eta_{TT} \eta_T^* \psi(x).$$
(1.334)

Hence  $\eta_{TT}\eta_T^* = -1$ . So, relative sign between  $\eta_{TT}$  and  $\eta_T$  must be -1. Since in experiments it is always a relative intrinsic parity between two wave functions that is measured (and not the phase factor itself), one conventionally chooses  $\eta_{TT} = i\eta_{TT}^R$  and  $\eta_T = i\eta_T^R$  with  $\eta_{TT}^R = \pm 1$  and  $\eta_T^R = \pm 1$ . With this convention we can finally write

$$\psi_T(x) = i\eta_T^R \gamma^1 \gamma^3 \psi^*(x_T), \qquad (1.335)$$

where  $\eta_T^R$  is *intrinsic time reversal*, i.e., another quantum number of the particle (akin to charge or spin). Instead of  $\eta_T^R$  one simply writes only  $\eta_T$ . Aside from  $\eta_T$  one can also check that

$$B^t = -B, \quad B^* = -B^{-1}.$$
 (1.336)

As an example we now compute a time reversal of the bispinor  $u(p, \lambda)$ .

This can be done as follows. We first write

$$\psi_{T}^{(+)}(x,p) = \boldsymbol{B} \left( u(p,\lambda)e^{-ipx_{T}} \right)^{*}$$

$$= i\eta_{T}\sqrt{E+m} \begin{pmatrix} i\sigma^{2} & 0\\ 0 & i\sigma^{2} \end{pmatrix} \begin{pmatrix} \chi_{\lambda}^{*} \\ \frac{p\cdot\sigma^{*}}{E_{T}+m}\chi_{\lambda}^{*} \end{pmatrix} e^{-ip_{T}x}$$

$$= i\eta_{T}\sqrt{E_{T}+m} \begin{pmatrix} i\sigma^{2}\chi_{\lambda}^{*} \\ \frac{-p\cdot(i\sigma^{2})\sigma^{*}(i\sigma^{2})}{E_{T}+m}i\sigma^{2}\chi_{\lambda}^{*} \end{pmatrix} e^{-ip_{T}x} . \quad (1.337)$$

Now we can use the fact that  $(\sigma^3/2 \text{ is a spin projection operator to } z$ -direction)

$$\frac{\sigma^3}{2}i\sigma^2\chi_{\lambda}^* = -\left(\frac{\sigma^3}{2}i(\sigma^2)^*\chi_{\lambda}\right)^* = \left(\frac{\sigma^3}{2}i\sigma^2\chi_{\lambda}\right)^*$$
$$= -\left(i\sigma^2\frac{\sigma^3}{2}\chi_{\lambda}\right)^* = -\lambda\left(i\sigma_{\lambda}^{\chi}\right)^* = -\lambda i\sigma^2\chi_{\lambda}^*. \quad (1.338)$$

Eq. (1.338) implies that  $i\sigma^2 \chi^*_{\lambda} \propto \chi_{-\lambda}$ . By employing the identity  $(i\sigma^2)\sigma^*(i\sigma^2) = \sigma$  we can rewrite (1.337) in the form

$$u_{T}(p,\lambda) = i\eta_{T}(-1)^{1/2+\lambda}\sqrt{E_{T}+m} \begin{pmatrix} \chi_{-\lambda} \\ \frac{p_{T}\cdot\sigma}{E_{T}+m}\chi_{-\lambda} \end{pmatrix}$$
$$= i\eta_{T}(-1)^{1/2+\lambda}u(p_{T},-\lambda).$$
(1.339)

Note that if one is interested only on a relative phase factor between different spin components, then (1.339) can be reduced to the relation

$$u_T(p,\lambda) = i(-1)^{1/2+\lambda} u(p_T, -\lambda) \equiv i\eta_\lambda u(p_T, -\lambda).$$
(1.340)

In this case the condition  $\eta_{TT}\eta_T^* = -1$  reduces to  $\eta_\lambda \eta_{-\lambda} = -1$ .

#### Time reversal of a Scalar Particle

For a complex wave function  $\phi(x)$  of a relativistic scalar (Klein-Gordon) particle

$$\phi(x) \to \eta_T \phi_T(x),$$

with  $\phi_T(x) = \phi(x_T)^*$ . Consistency of this prescription can be confirmed by looking at a state with a definite momentum  $\phi(p, x) = e^{-ipx}$ . In this case the prescription gives

$$\phi_T(p,x) = \{e^{-ipx_T}\}^* = e^{-ip_Tx} = \phi(p_T,x).$$

#### **Charge Conjugation**

Last of discrete symmetries we will discuss is a *charge conjugation C*, which simply accounts for a change of electric charge to its negative value, i.e.

$$q \xrightarrow{C} -q$$
. (1.341)

Note that charge conjugation is not a discrete symmetry of Lorentz group, though, there is a deep connection with the Lorentz symmetry via the so-called CPT theorem.

In the standard representation  $\chi_{\lambda}$  are real and it is easy to see that  $i\sigma^2\chi_{\lambda} = \chi_{-\lambda}(-1)^{1/2+\lambda}$ .

The issue of charge conjugation is best discussed when electromagnetic field is coupled to a charged particle via minimal coupling, i.e.

$$\left[\left(i\partial - qA\right) - m\right]\psi(x) = 0. \tag{1.342}$$

Charge conjugated wave function  $\psi_c(x)$  must satisfy

$$\left[\left(i\partial \!\!\!/ + qA\right) - m\right]\psi_c(x) = 0. \tag{1.343}$$

Note that from (1.342) directly follows that

$$\psi^{\dagger}(x)\left[-i\gamma^{\mu,\dagger}\overleftarrow{\partial_{\mu}}-q\gamma^{\mu,\dagger}A_{\mu}-m\right] = 0. \qquad (1.344)$$

By multiplying this equation from right by  $\gamma^0$  and using relation  $\gamma^0 \gamma^{\dagger} \gamma^0 = \gamma$ , we get

$$0 = \psi^{\dagger}(x)\gamma^{0} \left[ -i\gamma^{\mu} \overleftrightarrow{\partial_{\mu}} - q\gamma^{\mu}A_{\mu} - m \right]$$
$$= \overline{\psi}(x) \left[ -i\gamma^{\mu} \overleftrightarrow{\partial_{\mu}} - q\gamma^{\mu}A_{\mu} - m \right],$$
$$\Leftrightarrow \qquad \left[ -i(\gamma^{\mu})^{t}\partial_{\mu} - q(\gamma^{\mu})^{t}A_{\mu} - m \right] \overline{\psi}^{t}(x) = 0. \quad (1.345)$$

We might thus take the charge-conjugated Dirac's wave function in the form

$$\psi_c(x) = C\overline{\psi}'(x). \tag{1.346}$$

The matrix *C* must be chosen so that  $\psi_c$  satisfies Dirac equation with opposite charge. From all above we get that

$$\left(-iC(\gamma^{\mu})^{t}C^{-1}\partial_{\mu} - qC(\gamma^{\mu})^{t}C^{-1}A_{\mu} - m\right)\psi_{c}(x) = 0.$$
 (1.347)

Assuming that *C* satisfies

$$C(\gamma^{\mu})^{t}C^{-1} = -\gamma^{\mu}, \qquad (1.348)$$

we get from (1.345) that

$$\left(i\gamma^{\mu}\partial_{\mu} + q\gamma^{\mu}\partial_{\mu} - m\right)\psi_{c}(x) = \left(i\partial + qA - m\right)\psi_{c}(x) = 0, \ (1.349)$$

provided  $\psi(x)$  satisfies (1.342) (or equivalently (1.345)).

As for the matrix *C*, it can be checked that

$$\boldsymbol{C} = i\gamma^0\gamma^2 = \begin{pmatrix} 0 & i\sigma_2 \\ i\sigma_2 & 0 \end{pmatrix}. \tag{1.350}$$

#### C Matrix in Weyl/Chiral Representation

It can be checked that in Weyl/chiral representation the *C* matrix is

Existence of such matrix C is guaranteed by the Fundamental theorem of Clifford algebra.

In some convention **C** is taken as  $i\gamma^2\gamma^0$ , which differs by sign.

given by

$$\boldsymbol{C} = i \begin{pmatrix} 0 & \mathbf{1} \\ \mathbf{1} & 0 \end{pmatrix} \begin{pmatrix} 0 & \sigma_2 \\ -\sigma_2 & 0 \end{pmatrix} = \begin{pmatrix} -i\sigma_2 & 0 \\ 0 & i\sigma_2 \end{pmatrix}.$$

Note that

$$C = -C^{-1} = -C^{\dagger} = -C^{t}. \qquad (1.351)$$

 $\psi_c(x)$  describes particle with the same mass and the same spin direction, but with opposite charge and energy. *Change conjugation is antilinear transformation*.

Let us now compute  $\psi_c(x)$  for  $\psi(x)$  describing a spin-down negative energy electron at rest in absence of external field. Begin with (we omit the normalization factor  $\sqrt{2m}$ )

$$\psi(x) = e^{imt} \begin{pmatrix} 0\\0\\0\\1 \end{pmatrix},$$
 (1.352)

and take  $C = i\gamma^2\gamma^0$ . Then  $\psi_c(x)$  can be written as

$$\begin{split} \psi_{c}(x) &= \eta_{c} \boldsymbol{C} \overline{\psi}^{t} = i \eta_{c} \gamma^{2} \gamma^{0} (\psi^{\dagger}(x) \gamma^{0})^{t} \\ &= \eta_{c} \boldsymbol{C} (\gamma^{0})^{t} \gamma^{*}(x) = \eta_{c} (-\gamma^{0}) \boldsymbol{C} \psi^{*}(x) \\ &= \eta_{c} (-\gamma^{0}) i \gamma^{2} \gamma^{0} e^{-imt} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix} = \eta_{c} e^{-imt} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \quad (1.353) \end{split}$$

Therefore, charge conjugation of a negative-energy spin-down electron is equivalent to positive-energy spin-up solution. We thuse see that the spinor  $v(p, \lambda)$  is associated with the anti-particle. This connection will be discussed in some detail in the following section when Dirac's hole theory will be considered.

#### Full Lorentz Group — Brief Summary

- ► Lorentz transformations  $x^{\mu} \rightarrow x'^{\mu} = L^{\mu}_{,\nu} x^{\nu}$  preserve the invariance of the space-time interval  $x^{\mu}x_{\mu} = x'^{\mu}x'_{\mu}$ .
- This constraints the matrices  $L^{\mu}_{,\nu}$  to obey

$$L^{\mu}_{\alpha}\eta_{\mu\nu}L^{\nu}_{\ \beta} = \eta_{\alpha\beta} \quad \Leftrightarrow \quad \eta = L^{T}\eta L.$$

where  $\eta_{\mu\nu} = \text{diag}(-1, 1, 1, 1)$ .

• Condition  $\eta = L^T \eta L$  allows classification of transformations depending on whether

det 
$$L = \pm 1$$
 and  $L^0_{.0} = \pm \left[1 + \sum_i (L^i_{.i})^2\right]^{1/2}$ 

► Consequently, the full Lorentz group splits into 4 pairwise disjoint and non compact connected sets:

$$\mathcal{L}_{+}^{\uparrow}: \quad \det L = 1, \quad L_{.0}^{0} \ge 1,$$
$$\mathcal{L}_{-}^{\uparrow}: \quad \det L = -1, \quad L_{.0}^{0} \ge 1,$$
$$\mathcal{L}_{+}^{\downarrow}: \quad \det L = 1, \quad L_{.0}^{0} \le 1,$$
$$\mathcal{L}_{-}^{\downarrow}: \quad \det L = -1, \quad L_{.0}^{0} \le 1.$$

The transformation matrices *L* in  $\mathcal{L}^{\uparrow}_{+}$  form a soubgroup — *the* proper orthochronous Lorentz group (or restricted Lorentz group). All other transformations in the *full Lorentz group* can be obtained from  $L \subset \mathcal{L}^{\uparrow}_{+}$  by using two discrete transformations

- ► Parity :  $P^{\mu}_{,\nu} = \eta_{\mu\nu}$ ► Time Reversal:  $T^{\mu}_{,\nu} = -\eta_{\mu\nu}$ .

Clearly if  $L \subset \mathcal{L}^{\uparrow}_{+}$  then  $PL \subset \mathcal{L}^{\uparrow}_{-}$ ,  $TL \subset \mathcal{L}^{\downarrow}_{-}$  and  $PTL \subset \mathcal{L}^{\downarrow}_{+}$ .



Remarkably, nature is invariant under the proper orthochronous Lorenzt group  $\mathcal{L}^{\uparrow}_{+}$  but *not* under the full Lorentz group.

- ▶ Parity is *violated* in the weak interactions.
- ▶ Time reversal is *violated* in *K*-meson (kaon), *B*-meson and D-meson decays. It is also theoretically present in theory of strong interactions (quantum chromodynamics — QCD).

## 1.13 Dirac's Hole Theory and Positron

Although we have found that the Dirac theory accommodates negative energy solutions whose existence should not be ignored, we have as yet not examined the physical significance of those solutions.

According to quantum theory of radiation, an excited atomic state can lose its energy discontinuously by spontaneously emitting a photon, even in absence of any external field — this is why all atomic states (save for the ground state) have *finite live time* and due to  $\Delta t \Delta E \ge \hbar/2$ also *finite energy width*.

In the Dirac theory, however, the so-called ground state of an atom is not really the lowest energy state since there exists a continuum of negative-energy states from  $-mc^2$  to  $-\infty$ . This remains to be true even in cases when a Coulomb potential is included. Indeed, the minimal substitution implies at the classical level that

$$E = \pm \sqrt{(p - eA)^2 c^2 + m^2 c^4} + e\phi c , \qquad (1.354)$$

In zero magnetic field A = 0 and the maximum energy for the negative energy spectrum

$$E_{\max}^{<} = -mc^{2} + e\phi_{\max}c = -mc^{2}.$$
 (1.355)

In addition  $E^{<}$  is clearly unbounded from below as  $\phi \leq 0$ .

We know that an excited atomic state makes a radiative transition to the *ground state*. Similarly, we might expect that atomic electron in the ground state with energy  $mc^2 - E_{BE}$  (here  $E_{BE}$  is a binding energy) can emit spontaneously a photon of a sufficient energy that will allow the electron to bridge the energy gap to negative-energy states. Furthermore, once it reaches a negative energy states, it will keep on lowering its energy indefinitely. This scenario leads to the socalled *radiation catastrophe*, i.e., atom would radiate as "crazy" without ever attaining a stable state. Since we know that the ground state of the atom is stable, one must somehow prevent a catastrophic transition to states of  $E^{<}$ .

In 1930 Dirac proposed that all states within  $E^{<}$  are completely filled under normal conditions. Since the subsequent Dirac's argument can be easily understood by considering only a free particle, we confine our following discussion to spin-1/2 free particle. To this end we assume that *real electrons* are described solely by positive-energy states. These are the states with  $E = \sqrt{p^2 + m^2}$ . All states of negative energy are occupied by electrons — one electron in each state of negative energy with given p and spin projection  $\lambda$ . In this way a real electron of positive energy is prevented from falling into energetically lower and lower states by radiation emission. Hence, the radiation catastrophe is averted by Pauli's exclusion principle, which prevents these transitions.

In absence of any field (electromagnetic, etc.) the *vacuum* represents the negative energy ( $E^{<}$ ) continuum (so-called *Dirac sea*), whose states are completely occupied with electrons. Occasionally one of the negative-energy electrons in the Dirac sea can absorb a photon of energy  $\hbar \omega \ge 2mc^2$  and transit into positive energy states. As a result, a *hole* is created in Dirac sea. One might naturally ask, what is the meaning of such a hole in the occupied "sea" of negative states.

Even though the spectrum of energies is identical with Klein-Gordon particle, a non-existence of Pauli exclusion principle for scalar particles means that no Dirac's sea can be formed.



**Figure 1.3:** Formation of a hole within Dirac's sea.

The observable energy of the Dirac sea with a single hole in it is

$$E_{obs} = E_{vac} - (-|E_e|) = E_{vac} + |E_e|.$$
(1.356)

So,  $E_{vac}$  has increased, hence we expect that the absence of a negativeenergy electron appears as the presence of a positive-energy particle, a *hole*.

Similarly, when a hole is created in Dirac's sea, the total charge of the Dirac's sea becomes

$$Q_{obs} = Q_{vac} - e = Q_{vac} - (-|e|) = Q_{vac} + |e|.$$
(1.357)

Thus, a hole in the sea of negative-energy states looks like a positiveenergy particle of charge |e|.

Once we accept that (*a*) negative-energy are completely filled under normal conditions, (*b*) negative-energy electron can absorb a photon of energy  $\hbar \omega > 2mc^2$  (just like a positive-energy electron can) to become a positive-energy electron, we are unambiguously led to the existence of a particle of a charge |e| with a positive energy. This particle is called *positron*. The absorption of two-photon quanta by a negative-energy electron can be formally written as

$$e_{E<0}^- + 2\gamma \to e_{E>0}^-$$
, (1.358)

We may also consider a closely related process when a positive-energy emits photon and falls to the negative-energy sea, i.e.

$$e_{E>0}^- + e_{E>0}^+ \to 2\gamma$$
, (1.359)

which is allowed only when a hole is present in Dirac's sea. Process (1.359) basically describes that both electron and hole/positron disappear and two photon quanta are generated. This process, called  $e^-e^+$  annihilation is often observed in solids.

We can gain further information on hole/positron by looking on its momentum  $p_{hole}$ . Again, absence of *momentum*  $p^e$  in the Dirac sea appears as a presence of  $-p^e$  momentum of a hole. Indeed

$$\boldsymbol{p}_{obs} = \boldsymbol{p}_{vac} - \boldsymbol{p}^e, \qquad (1.360)$$

Positron was experimentally discovered by Carl David Anderson on 2 August 1932, by observing cosmic rays in a cloud chamber (the Nobel Prize for Physics in 1936). Name *positron* first appeared in his paper.

Note that a single  $\gamma$  quantum (SQA) annihilation is forbidden, for real processes, for a free  $e^-e^+$  pair, due to the impossibility of balancing both momentum and energy conservation simultaneously. The most probable is the creation of two or more photon quanta. Nonetheless, in the presence of a third body, e.g., a nucleus in atom, SQA is allowed since the third body can recoil and allow simultaneous momentum and energy conservation. or equivalently the momentum of hole/positron is

$$p_{hole} = p_{obs} - p_{vac} = -p^e$$
. (1.361)

Similarly, one can argue that the absence of spin up for E < 0 electron is manifested as a presence of spin down of E > 0 positron. These conclusions can be summarise in the following table below. In the table

	Q	E	p	$\hat{\sigma}$	h
E < 0 electron state	- e	- E	p	$\frac{\hbar}{2}\Sigma$	$\frac{1}{2}\Sigma \cdot \frac{p}{ p }$
positron state	+ e	+ E	- <i>p</i>	$-\frac{\hbar}{2}\Sigma$	$\frac{\overline{1}}{2}\Sigma \cdot \frac{p}{ p }$

**Table 1.2:** Comparison of properties ofnegative-energy electron and ensuingpositive-energy hole/positron

we have introduces the notion of *helicity* 

$$\boldsymbol{h} = \frac{1}{2} \boldsymbol{\Sigma} \cdot \frac{\boldsymbol{p}}{|\boldsymbol{p}|}, \qquad (1.362)$$

i.e., projection of the spin along the direction of particle's 3-momentum.

#### "Helicity"

Sometimes the choice of the Pauli spinors

$$\chi_{\frac{1}{2}} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$$
 and  $\chi_{-\frac{1}{2}} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ ,

with the particle spin quantized along the *z*-axis is not the most convenient basis in the spinor space. Instead of the *z*-axis, one can choose any quantization direction. Particularly special is the situation when the direction is chosen to be along particle's 3-momentum p.

It should be noted that the spin operator  $\hat{\sigma} = \frac{1}{2}\Sigma$  does not commute with free Dirac's Hamiltonian  $H_D$ . In fact,

$$[H_D,\hat{\sigma}] = i\alpha \times p \neq 0,$$

where  $\alpha$  is Dirac's  $\alpha$ -matrix (see, Eq. (1.63)).

So far, the index  $\lambda$  in Dirac's bispinors referred to spin projection along *z*-axis in the rest frame. Since the *z*-axis spin projection is not conserved under time evolution, it is better to label the bispinor with another intrinsic quantum number that preserves a spin projection under time evolution. *Helicity h* provides such a quantum number. Indeed, since **p** commutes with Dirac's free Hamiltonian we have

$$[H_D, \boldsymbol{h}] = i(\boldsymbol{\alpha} \times \boldsymbol{p}) \cdot \frac{\boldsymbol{p}}{|\boldsymbol{p}|} = 0.$$

Here we used the identity  $(A \times B) \cdot C = (B \times C) \cdot A$ .

It can be also easily checked that

$$h^{2} = \frac{(\hat{\sigma} \cdot p)(\hat{\sigma} \cdot p)}{|p|^{2}} = \frac{\{\hat{\sigma}_{i}, \hat{\sigma}_{j}\}p_{i}p_{j}}{2|p|^{2}} = \frac{1}{4}$$

So, by Hamilton-Cayley theorem the eigenvalues of h are  $\pm 1/2$ . Particles with helicity  $\pm 1/2$  are conventionally referred as *right*-*handed*, and those with -1/2 are *left-handed*.

Note that (free) right-handed and left-handed particle states retain their identity under the boosts only if they are massless, because only in massless case it is impossible to change particle's helicity by bringing it to rest frame and reversing its direction of motion.

In passing we might notice that the charge conjugate negative-energy solutions presented in Section 1.12 have all traits that are possessed by hole/positrons (cf. Table 1.2). In other word, positrons can be identified with charge conjugate negative-energy electrons.

## 1.14 Antiparticles

On the basis of our previous discussion, it would seem that only fermions (specifically spin-1/2 fermions) can have antiparticles. It is, however, a striking feature of relativistic quantum theory that it naturally ensures existence of antiparticle to any kind of particle (be it boson or fermion). Though, Quantum Field Theory provides more natural framework for discussing this issue, the essence can be already understood in the context of relativistic quantum mechanics.

To understand what is involved, let us observe that Lorentz transformations do not necessarily leave invariant the order of events. For instance, suppose that event at  $x_2$  occurs later that at  $x_1$ , i.e.  $x_0^2 > x_0^1$ . A second observer who sees the first observer moving with velocity vwill see the events separated by time difference

$$\mathbf{x}_{2}^{'0} - \mathbf{x}_{1}^{'0} = \mathbf{L}_{i}^{0}(\mathbf{v})(\mathbf{x}_{2}^{i} - \mathbf{x}_{1}^{i}), \qquad (1.363)$$

For boosts in generic velocity direction one has

$$L^{i}{}_{j} = \delta^{i}_{j} = v_{i}v_{j}\frac{(\gamma-1)}{v^{2}},$$
  

$$L^{0}{}_{i} = -\gamma v_{i},$$
  

$$L^{0}{}_{0} = \gamma, \quad \gamma = (1-v^{2})^{-1/2}$$

or more explicitly

$$\boldsymbol{x}_{2}^{\prime 0} - \boldsymbol{x}_{1}^{\prime 0} = \gamma(\boldsymbol{x}_{2}^{0} - \boldsymbol{x}_{1}^{0}) - \gamma \boldsymbol{\nu}(\boldsymbol{x}_{2} - \boldsymbol{x}_{1}). \quad (1.364)$$

This is *negative* if

$$\mathbf{v}(\mathbf{x}_2 - \mathbf{x}_1) > (\mathbf{x}_2^0 - \mathbf{x}_1^0),$$
 (1.365)

which provides a seeming causality paradox. In fact, suppose that 1st observer sees a radioactive decay  $A \rightarrow B + C$  at  $x_1$ , followed by absorption of particle B, e.g.  $B + D \rightarrow E$  at  $x_2$ .



Will then the 2nd observer see *B* particle absorbed at  $x_2$  before it is emitted at  $x_1$ ?

This paradox disappears if we note that the speed  $|v| \le 1$ , so that we can write

$$(\mathbf{x}_{2}^{0} - \mathbf{x}_{1}^{0}) < \mathbf{v}(\mathbf{x}_{2} - \mathbf{x}_{1}) = |\mathbf{v}(\mathbf{x}_{2} - \mathbf{x}_{1})| \le |\mathbf{v}||(\mathbf{x}_{2} - \mathbf{x}_{1})|$$
  
$$\Rightarrow \quad (\mathbf{x}_{2}^{0} - \mathbf{x}_{1}^{0}) < |(\mathbf{x}_{2} - \mathbf{x}_{1})|. \quad (1.366)$$

This is clearly impossible because to travel from  $x_1$  to  $x_2$  would require the average velocity greater than 1 (that is > c), since

=

$$\frac{|\mathbf{x}_2 - \mathbf{x}_1|}{(\mathbf{x}_2^0 - \mathbf{x}_1^0)} > 1.$$
 (1.367)

Consequently, temporal order raises no problem in classical physics, but it plays an important role in quantum theories.

In fact, in quantum theory the uncertainty principle tells us that when we specify that a particle is at position  $x_1$  at time  $t_1$ , we cannot also define its velocity precisely. Consequently, there is a certain chance of particle getting from  $x_1$  to  $x_2$  even if  $x_1$  and  $x_2$  are space-like separated, i.e.  $|x_1 - x_2| > |x_1^0 - x_2^0|$ .

To be more precise, from quantum mechanical commutation relations one can derive that under Lorentz transformations [we set  $(t_1, x_1) = (0, 0)$  and  $(t_2, x_2) = (t, x, 0, 0)$ ]

$$(x_1' - x_2')^2 = ct'^2 - x'^2 = c^2 t^2 - x^2 + \hbar^2 c^2 \hat{H}^{-2}/4, \qquad (1.368)$$

where  $\hat{H}^2 = p^2 c^2 + m^2 c^4$  and both p and x are quantum mechanical operators with the usual canonical commutation relations. So, *quantum-mechanical Lorentz transformations* (in contrast to classical ones) *do not* generally *preserve* the notion of *time-like*, *space-like* or *light-like separation* under Lorenzt transformation. Indeed, let us start with *time-like* (or *light-like*) interval  $c^2 t'^2 - x'^2$ . Since  $\hat{H}^2 \ge m^2 c^4$  (in the sense of eigenvalues or quantum-mechanical averages), we get for such a time-like (or

**Figure 1.4:** A radioactive decay  $A \rightarrow B + C$  at  $x_1$ , followed by absorption of particle *B*, e.g.  $B + D \rightarrow E$  at  $x_2$ .

Note that temporal order can only be affected if the events  $x_1$  and  $x_2$  are *space-like separated*, i.e., when:

$$(x_1 - x_2)^{\mu} (x_1 - x_2)_{\mu} < 0$$

Space-like, time-like and light-like separations are Lorentz invariant concepts.

See, e.g., Zhi-Yong Wang and Cai-Dong Xiong, Physics Letters B 659 (2008) 707–711. light-like) interval that

$$0 \leq c^{2}t^{'2} - \mathbf{x}^{'2} = c^{2}t^{2} - \mathbf{x}^{2} + \hbar^{2}c^{2}\frac{\hat{\mathbf{H}}^{-2}}{4}$$
$$\leq c^{2}t^{2} - \mathbf{x}^{2} + \frac{\hbar^{2}}{4m^{2}c^{2}}$$
$$= c^{2}t^{2} - \mathbf{x}^{2} + \left(\frac{\hbar}{2}\right)^{2}. \quad (1.369)$$

Here  $\lambda = \frac{\hbar}{mc}$  is the (reduced) Compton wavelength of the particle. Consequently, the particle in the "unprimed" frame can propagate over *space-like* interval provided that

$$0 > c^{2}t^{2} - x^{2} \ge -\left(\frac{\hbar}{2}\right)^{2}.$$
 (1.370)

So, we see that the notion of time-like separation is not conserved in quantum mechanics.

Inequality (1.370) is particular version of the so-called *Weinberg formula*, which has a general form

$$0 > c^{2}(t_{2} - t_{1})^{2} - (\mathbf{x}_{1} - \mathbf{x}_{2})^{2} \ge -\left(\frac{\lambda}{2}\right)^{2}.$$
 (1.371)

Such space time intervals are very "narrow" even for elementary particle masses, e.g. if *m* is the mass of electron, then  $\lambda = 3.9 \times 10^{-13}$ m. We are thus faced again with a paradox; if one observer sees a particle emitted at  $x_1$  and absorbed at  $x_2$ , and if the Weinberg formula is satisfied, then a second observer may see the particle absorbed at  $x_2$  at a time  $t_2$  before it is emitted at  $x_1$  at time  $t_1$ .



There is only one known way out of this paradox. The second observer must see a particle emitted at  $x_2$  and absorbed at  $x_1$ . But in general the particle seen by the second observer must necessarily be different from the first one.

Though in our preceding argument it was the "primed" frame where events were time-like and "unprimed" frame where events could be space-like, the illustrative figures have the role of frames reversed so that we could make easier connection with our earlier classical causal paradox.

**Figure 1.5:** Quantum causality paradox. Time-like intervals are not generally preserved under Lorentz transformations. The violation is quantified by Weinberg formula.


**Figure 1.6:** Antiparticles solve the quantum causality paradox.

For instance, if the first observer sees a proton turn into a neutron and positive  $\pi$ -meson at  $x_1$  and then sees  $\pi^+$  and some other neutron turn into proton at  $x_2$ , then the second observer must see the neutron at  $x_2$  turn into proton and a particle of a *negative* charge, which is then absorbed by a proton at  $x_1$  that turns into a neutron. Since the rest mass is a Lorentz invariant, the mass of the negative charged particle seen by the second observer will be equal to that of  $\pi^+$ . There is indeed experimentally observed such a particle and it is called negative  $\pi$ -meson (or shortly pion  $\pi^-$ ).

This analysis allows us to make the following general statement: For every type of charged particle there is an oppositely charged particle of equal mass. Note, that this conclusion is not obtainable in non-relativistic quantum mechanics, nor in relativistic classical mechanics.

#### "Feynman-Stueckelberg Interpretation of Antiparticles"

Uncertainty relations allow that a particle can "tunnel" from timelike to space-like regions. This situation is depicted at Fig. 1.6. By comparing both figures in Fig. 1.6 we can make the following identifications:

- in frame *II*: π<sup>−</sup> brings to the vertex x<sub>1</sub> a *positive energy* ↔ in frame *II*: π<sup>+</sup> leaves the vertex x<sub>1</sub> with a *negative energy*
- in frame *II*: π<sup>−</sup> brings to the vertex x<sub>1</sub> certain value of *spin* projection
  () in frame *U*: π<sup>+</sup> leaves the vertex x<sub>1</sub> with the emergine radius

 $\leftrightarrow$  in frame *II*:  $\pi^+$  leaves the vertex  $x_1$  with the *opposite value of spin projection* 

in frame *II*: π<sup>−</sup> brings to the vertex x<sub>1</sub> certain value of *helicity* ↔ in frame *II*: π<sup>+</sup> leaves the vertex x<sub>1</sub> with the *same value of helicity* (both spin and momenta are reversed).

Similar statements hold true also in connection with the vertex  $x_2$ .

Above parallelisms leads to the following *Feynman–Stueckelberg interpretation of antiparticles:* 

Antiparticle can be viewed as a particle with *negative energy*, *charge* and *spin* moving *backward* in time.

### 1.15 Central field problem: exact solution

One of the key successes of Dirac's theory was the correct prediction of a *fine structure* in the energy levels of hydrogen. In this section we will discuss the issue of a relativistic electron in a central potential with a particular emphasize on a Coulomb potential.

We start with an eigenvalue problem for Dirac's Hamiltonian describing a particle in a central scalar potential. This reads

$$H_D\psi = [\alpha \cdot \boldsymbol{p} + \beta m + V(r)]\psi = E\psi, \qquad (1.372)$$

where in the Dirac representation

$$\boldsymbol{\alpha} = \begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \quad \boldsymbol{\beta} = \begin{pmatrix} \mathbf{1} & 0 \\ 0 & -\mathbf{1} \end{pmatrix}. \tag{1.373}$$

An important observation in this context is that the *total angular momentum* 

$$J = r \times p + \hat{\sigma}, \qquad (1.374)$$

(and not not orbital angular momentum  $L = r \times p$  or spin  $\hat{\sigma}$  separately) is conserved.

#### Note on conserved quantities in Quantum Mechanics

Conserved quantity (say  $J_{\mu\nu}$ ) must transform state vector in the same spacetime point namely

$$\psi'(x) = e^{-\frac{i}{2}J_{\mu\nu}\omega^{\mu\nu}}\psi(x).$$
(1.375)

So, in particular  $J_{\mu\nu}$  can be easily read off from the linear  $\omega^{\mu\nu}$  term in the  $|\omega^{\mu\nu}| << 1$  expansion, where

$$\psi'(x) \sim \left(\mathbf{1} - \frac{i}{2}J_{\mu\nu}\omega^{\mu\nu}\right)\psi(x)$$

Reason why such  $J_{\mu\nu}$  should be conserved follows from the fact that

$$H\psi = E\psi \quad \Leftrightarrow \quad e^{-\frac{i}{2}J_{\mu\nu}\omega^{\mu\nu}}He^{\frac{i}{2}J_{\mu\nu}\omega^{\mu\nu}}e^{-\frac{i}{2}J_{\mu\nu}\omega^{\mu\nu}}\psi = Ee^{-\frac{i}{2}J_{\mu\nu}\omega^{\mu\nu}}\psi.$$

Now, if  $J_{\mu\nu}$  is conserved then  $[J_{\mu\nu}; H] = 0$ , this is, however, equivalent to the statement that

$$e^{-\frac{i}{2}J_{\mu\nu}\omega^{\mu\nu}}He^{\frac{i}{2}J_{\mu\nu}\omega^{\mu\nu}} = H,$$

which then implies that also

$$\psi'(x) = e^{-\frac{i}{2}J_{\mu\nu}\omega^{\mu\nu}}\psi(x)$$

is an eigenstate of the Hamiltonian with the same energy *E* as the state  $\psi(x)$ . Since this statement is true at the level of energy

eigenstates, it must be true also for any state vector since these these can be written as a linear combination of energy eigenstates.

We know that to the *linear* order in  $\omega^{\mu\nu}$ 

$$\begin{split} \psi'(x) &= S(L)\psi(L^{-1}x) \underbrace{\longmapsto}_{|\omega|<<1} \left(\mathbbm{1} - \frac{i}{4}\sigma_{\mu\nu}\omega^{\mu\nu}\right)\psi(L^{-1}x) \\ &= \left(\mathbbm{1} - \frac{i}{4}\sigma_{\mu\nu}\omega^{\mu\nu}\right)\psi(x^{\rho} - \omega^{\rho}{}_{\nu}x^{\nu}) \\ &= \left(\mathbbm{1} - \frac{i}{4}\sigma_{\mu\nu}\omega^{\mu\nu} - \underbrace{\omega^{\rho}{}_{\nu}x^{\nu}}_{\omega^{\rho\nu}x_{\nu}}\frac{\partial}{\partial x^{\rho}}\right)\psi(x) \\ &= \left[\mathbbm{1} - \frac{i}{4}\sigma_{\mu\nu}\omega^{\mu\nu} - \frac{1}{2}\omega^{\mu\nu}(x_{\nu}\partial_{\mu} - x_{\mu}\partial_{\nu})\right]\psi(x) \\ &= \left\{\mathbbm{1} - \frac{i}{2}\omega^{\mu\nu}\left[\frac{1}{2}\sigma_{\mu\nu} + i(x_{\mu}\partial_{\nu} - x_{\nu}\partial_{\mu})\right]\right\}\psi(x). \end{split}$$

So,

$$J_{\mu\nu} = \frac{1}{2}\sigma_{\mu\nu} + i(x_{\mu}\partial_{\nu} - x_{\nu}\partial_{\mu}),$$

is our candidate conserved quantity. Since the components  $J_{0i}$  are associated with boots, they cannot be conserved, i.e., they cannot commute with Hamiltonian  $H_D$ , since boosts inevitably change the value of energy. Thus, the only possible candidate conserved quantity can be  $J_{ij}$  (i, j = 1, 2, 3), which after contraction with  $\frac{1}{4}\varepsilon^{ijk}$  yields the total angular momentum (1.374).

In particular, neither  $\frac{1}{2}\sigma_{\mu\nu}$  nor  $i(x_{\mu}\partial_{\nu} - x_{\nu}\partial_{\mu})$  are conserved separately. Note that non of them separately transforms the state vector according to prescription (1.375).

The first thing to note is that  $\{H_D; J^2; J_z\}$  can be simultaneously diagonalized.

#### **Proof:**

Both in Weyl and Dirac representations of the matrix  $\hat{\sigma}$  is block diagonal with identical blocks and hence the angular momentum operator J acts in the same way on the upper and lower bispinor components

$$\boldsymbol{J}\boldsymbol{\psi} = \begin{pmatrix} \boldsymbol{L} + \frac{1}{2}\boldsymbol{\sigma} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{L} + \frac{1}{2}\boldsymbol{\sigma} \end{pmatrix} \begin{pmatrix} \boldsymbol{\psi}^+ \\ \boldsymbol{\psi}^- \end{pmatrix}, \qquad (1.376)$$

To compute the commutator  $[H_D, J]$  we turn for definiteness to Dirac's representation. In this case

$$[H_D, \boldsymbol{J}] = \begin{bmatrix} \left( \begin{bmatrix} V(r) + m \end{bmatrix} \mathbb{1}_{2 \times 2} & \boldsymbol{\sigma} \cdot \boldsymbol{p} \\ \boldsymbol{\sigma} \cdot \boldsymbol{p} & \begin{bmatrix} V(r) - m \end{bmatrix} \mathbb{1}_{2 \times 2} \right), \begin{pmatrix} \boldsymbol{L} + \frac{1}{2}\boldsymbol{\sigma} & \boldsymbol{0} \\ \boldsymbol{0} & \boldsymbol{L} + \frac{1}{2}\boldsymbol{\sigma} \end{pmatrix} \end{bmatrix}$$
$$= \underbrace{ \begin{bmatrix} \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta m, \hat{\boldsymbol{\sigma}} \end{bmatrix}}_{A} + \underbrace{ \begin{bmatrix} \boldsymbol{\alpha} \cdot \boldsymbol{p} + V(r), \boldsymbol{r} \times \boldsymbol{p} \end{bmatrix}}_{B}.$$
(1.377)

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The commutator "A" reduces to

$$\begin{pmatrix} m & \boldsymbol{\sigma} \cdot \boldsymbol{p} \\ \boldsymbol{\sigma} \cdot \boldsymbol{p} & m \end{pmatrix}, \begin{pmatrix} \frac{1}{2}\boldsymbol{\sigma} & 0 \\ 0 & \frac{1}{2}\boldsymbol{\sigma} \end{pmatrix} \end{bmatrix}$$

$$= \begin{pmatrix} \frac{m}{2}\boldsymbol{\sigma} & \frac{1}{2}(\boldsymbol{\sigma} \cdot \boldsymbol{p}) \cdot \boldsymbol{\sigma} \\ \frac{1}{2}(\boldsymbol{\sigma} \cdot \boldsymbol{p}) \cdot \boldsymbol{\sigma} & -\frac{m}{2}\boldsymbol{\sigma} \end{pmatrix} - \begin{pmatrix} \frac{m}{2}\boldsymbol{\sigma} & \frac{1}{2}\boldsymbol{\sigma} \cdot (\boldsymbol{\sigma} \cdot \boldsymbol{p}) \\ \frac{1}{2}\boldsymbol{\sigma} \cdot (\boldsymbol{\sigma} \cdot \boldsymbol{p}) & -\frac{m}{2}\boldsymbol{\sigma} \end{pmatrix}$$

$$= \begin{pmatrix} 0 & \frac{1}{2}[\boldsymbol{\sigma} \cdot \boldsymbol{p}; \boldsymbol{\sigma}] \\ \frac{1}{2}[\boldsymbol{\sigma} \cdot \boldsymbol{p}; \boldsymbol{\sigma}] & 0 \end{pmatrix} = \begin{pmatrix} 0 & \frac{1}{2}[\boldsymbol{\sigma}_i; \boldsymbol{\sigma}] p_i \\ \frac{1}{2}[\boldsymbol{\sigma}_i; \boldsymbol{\sigma}] p_i & 0 \end{pmatrix}$$

$$= i \begin{pmatrix} 0 & \boldsymbol{\sigma} \times \boldsymbol{p} \\ \boldsymbol{\sigma} \times \boldsymbol{p} & 0 \end{pmatrix} = i \boldsymbol{\alpha} \times \boldsymbol{p} .$$

$$(1.378)$$

Similarly, the commutator "B" can be written as

$$[\boldsymbol{\alpha} \cdot \boldsymbol{p} + V(r), \boldsymbol{r} \times \boldsymbol{p}] = \underbrace{[V(r), \boldsymbol{r} \times \boldsymbol{p}]}_{a} + \underbrace{[\boldsymbol{\alpha} \cdot \boldsymbol{p}, \boldsymbol{r} \times \boldsymbol{p}]}_{b}, \quad (1.379)$$

where the commutator "a" reads

$$[V(r), \mathbf{r} \times \mathbf{p}]_{k} = \epsilon^{ijk} [V(r), r^{i}p^{j}] = \epsilon^{ijk} r^{i} [V(r), p^{j}]$$
$$= \epsilon^{ijk} r^{i} \left( i \frac{\partial}{\partial x^{j}} V(r) \right) = \epsilon^{ijk} \left( -\frac{ir^{i}r^{j}}{r} \frac{\partial V}{\partial r} \right) = 0, \quad (1.380)$$

and "b" is

$$[V(r), \mathbf{r} \times \mathbf{p}]_{k} = \alpha^{i} \epsilon^{lmk} [p^{i}, r^{l} p^{m}] = \alpha^{i} \epsilon^{lmk} [p^{i}, r^{l}] p^{m}$$
$$= -i\alpha^{i} \epsilon^{imk} p^{m} = -i(\boldsymbol{\alpha} \times \mathbf{p})_{k}.$$
(1.381)

By putting together all results obtained we get that indeed  $[H_D, J] = 0$ . This directly implies that also  $[H_D, J^2] = 0$  and  $[H_D, J_z] = 0$ . Since the algebra for the angular momentum ensures that  $[J^2, J_i] = 0$  for all i = 1, 2, 3 but  $[J_i, J_k] \neq 0$  for all  $i \neq j$ , we see that the triple of operators  $H_D$ ,  $J^2$  and  $J_z$  pairwise commute and hence  $\{H_D, J^2, J_z\}$  can be simultaneously diagonalized. This concludes the proof

A consequence of our previous analysis is that the Dirac spinor angular momentum eigenstates satisfy

$$J^{2}\psi = j(j+1)\psi; J_{3}\psi \equiv J_{z}\psi = m\psi \text{ with } m \in (-J, ..., J), (1.382)$$

and (due to a diagonal nature of J) they must be composed of twocomponent Pauli spinors with the same angular momentum eigenvalues, i.e.,  $\psi$  from (1.382) can be written as

$$\psi = \begin{pmatrix} \psi^+ \\ \psi^- \end{pmatrix} = \begin{pmatrix} \varphi_{j,m} \\ \chi_{j,m} \end{pmatrix}.$$
(1.383)

Note that we have already observed this type of behavior in the case of a free Dirac particle with spin in place of total angular momentum.

There is yet another operator that commutes with  $H_D$  and J. Intuitively, we expect that we must be able to specify whether the electron spin is parallel or antiparallel to the total angular momentum. In

non-relativistic Quantum Mechanics these two possibilities would be distinguished by the eigenvalues of the operator

$$\boldsymbol{\sigma} \cdot \boldsymbol{J} = \boldsymbol{\sigma} \left( \boldsymbol{L} + \frac{\boldsymbol{\sigma}}{2} \right) \,. \tag{1.384}$$

For a relativistic electron we might try a  $4 \times 4$  generalization of (1.384), namely  $\Sigma \cdot J$  or  $\hat{\sigma} \cdot J$ . It can be, however, checked that this would not work.

Recall that  $\Sigma = 2\hat{\sigma}$ 

One might thus try  $\beta \Sigma \cdot J$ , which has the same non-relativistic limit as  $\Sigma \cdot J$ . In this case

$$[H_D, \beta \hat{\boldsymbol{\sigma}} \cdot \boldsymbol{J}] = \frac{1}{4} [H_D; \beta] \quad \text{or} \quad [H_D, \beta \boldsymbol{\Sigma} \cdot \boldsymbol{J}] = \frac{1}{2} [H_D, \beta]. \quad (1.385)$$

The proof of this statement is quite straightforward. First we might observe that

$$[H_D, \beta \Sigma \cdot J] = [H_D, \beta] (\Sigma \cdot J) + \beta [H_D, \Sigma \cdot J]$$
$$= -2\beta (\alpha \cdot p) (\Sigma \cdot J) + 2i\beta (\alpha \times p) \cdot J. \quad (1.386)$$

Now, in Dirac's representation we have

$$(\boldsymbol{\alpha} \cdot \boldsymbol{p})(\boldsymbol{\Sigma} \cdot \boldsymbol{J}) = (\sigma^{1} \otimes \boldsymbol{\sigma} \cdot \boldsymbol{p})(\mathbb{1} \otimes \boldsymbol{\sigma} \cdot \boldsymbol{J})$$
  
$$= [\sigma^{1} \otimes (\boldsymbol{\sigma} \cdot \boldsymbol{p})(\boldsymbol{\sigma} \cdot \boldsymbol{J})] = \sigma^{1} \otimes \sigma^{i} \sigma^{j} p^{i} J^{j}$$
  
$$= \sigma^{1} \otimes (\delta^{ij} + i\epsilon^{ijk} \sigma^{k}) p^{i} J^{j}$$
  
$$= \underbrace{(\sigma_{1} \otimes \boldsymbol{p} \cdot \boldsymbol{J})}_{\gamma^{5} \boldsymbol{p} \cdot \boldsymbol{J}} + i \underbrace{[\sigma_{1} \otimes \boldsymbol{\sigma} \cdot (\boldsymbol{p} \times \boldsymbol{J})]}_{i\boldsymbol{\alpha} \cdot (\boldsymbol{p} \times \boldsymbol{J})}, \quad (1.387)$$

This finally implies that

$$[H_D, \beta \Sigma \cdot J] = -2\beta \gamma^5 p \cdot J - 2\beta [[i\alpha \cdot (p \times J)] + 2i\beta(\alpha \times p) \cdot J]$$
$$= -2\beta \gamma^5 p \cdot J = -2\beta \gamma^5 \left[ p \cdot \left( L + \frac{\Sigma}{2} \right) \right] = -2\beta \gamma^5 p \cdot \frac{\Sigma}{2}$$
$$= -2\beta \left( \sigma_1 \otimes \frac{\sigma}{2} \right) \cdot p = -\beta \alpha \cdot p = \frac{1}{2} [H_D, \beta]. \quad (1.388)$$

This result [see also Eq. (1.385)] indicates that we can define a new operator *K*:

$$K = \beta \Sigma \cdot J - \frac{\beta}{2} = \beta \left[ \Sigma \left( L + \frac{\Sigma}{2} \right) - \frac{1}{2} \right] = \beta \left( \Sigma L + \frac{\Sigma^2}{2} - \frac{1}{2} \right)$$
$$= \beta \left( \Sigma L + \frac{3}{2} - \frac{1}{2} \right) = \beta (\Sigma L + 1), \qquad (1.389)$$

which commutes with  $H_D$ , i.e.,  $[H_D; K] = 0$ . Furthermore, since J commutes with  $\beta$  and  $\Sigma \cdot L$  then also [J, K] = 0 and hence  $[J^2, K] = 0$ . Consequently, for Dirac's particle in a central potential we can construct a simultaneous eigenfunctions of  $H_D$ ; K;  $J^2$  and  $J_z$ . The corresponding eigenvalues will be further denoted as E,  $-\kappa$ , j(j + 1) and m, respectively. It should be noted that  $\kappa$  and j are not totally independent (similarly as m and j are not). To see how they are related let us consider  $K^2$ , this gives

$$K^{2} = \beta(\Sigma \cdot L + 1)\beta(\Sigma \cdot L + 1) = \beta^{2}(\Sigma \cdot L + 1)^{2}$$

$$= (\Sigma \cdot L)(\Sigma \cdot L) + 2\Sigma \cdot L + 1$$

$$= \begin{pmatrix} \sigma^{i} & 0 \\ 0 & \sigma^{i} \end{pmatrix} \begin{pmatrix} \sigma^{j} & 0 \\ 0 & \sigma^{j} \end{pmatrix} L_{i}L_{j} + 2\Sigma \cdot L + 1$$

$$= L^{2} + i\Sigma^{k}\epsilon^{ijk}L_{i}L_{j} + 2\Sigma L + 1$$

$$= L^{2} - \Sigma L + 2\Sigma L + 1 = L^{2} + \Sigma L + 1. \quad (1.390)$$

At the same time we have

$$J^{2} = \left(L + \frac{\Sigma}{2}\right)^{2} = L^{2} + \frac{2}{2}\Sigma \cdot L + \frac{\Sigma^{2}}{4} = L^{2} + \Sigma \cdot L + \frac{3}{4}, \quad (1.391)$$

so, we can write  $K^2 = J^2 + \frac{1}{4}$ . Thus, eigenvalues  $J^2$  and  $K^2$  are related to each other by the relation

$$\kappa^2 = j(j+1) + \frac{1}{4} = \left(j + \frac{1}{2}\right)^2,$$
(1.392)

or in other words,  $\kappa = \pm \left(j + \frac{1}{2}\right)$ . Since  $j = 1/2, 3/2, 5/2, \ldots$  we see that  $\kappa$  is a *non-zero integer* which can be both positive and negative.

From (1.389) follows that *K* has an explicit form

$$K = \begin{pmatrix} \boldsymbol{\sigma}\boldsymbol{L} + 1 & 0\\ 0 & -\boldsymbol{\sigma}\boldsymbol{L} - 1 \end{pmatrix} = \begin{pmatrix} \boldsymbol{\sigma}\boldsymbol{J} - \frac{1}{2} & 0\\ 0 & -\boldsymbol{\sigma}\boldsymbol{J} + \frac{1}{2} \end{pmatrix}.$$
(1.393)

#### Note:

Pictorially speaking, the sign of  $\kappa$  determines whether the spin is *antiparallel* ( $\kappa > 0$ ) or *parallel* ( $\kappa < 0$ ) to **J** in the non-relativistic limit.

So, if Dirac's wave function  $\psi$  (assumed to be an energy eigenfunction) is a simultaneous eigenfunction of *K*,  $J^2$  and  $J_z$  then it must satisfy

$$\underbrace{(\sigma L+1)\psi_{+} = -\kappa\psi_{+}, \quad (\sigma L+1)\psi_{-} = \kappa\psi_{-}}_{K\psi = -\kappa\psi}, \quad (1.394)$$

and

$$J^{2}\psi_{\pm} = (L + \sigma/2)^{2}\psi_{\pm} = j(j+1)\psi_{\pm},$$
  
$$J_{z}\psi_{\pm} = (L_{3} + \sigma_{3}/2)^{2}\psi_{\pm} = m\psi_{\pm}.$$
 (1.395)

Note that the operator  $L^2 = J^2 - \Sigma \cdot L - \frac{3}{4}$  when acted on  $\psi_+$  and  $\psi_-$ 

Here we use the identity:  $\sigma^i \sigma^j = \delta^{ij} + i\epsilon^{ijk}\sigma^k$ . gives

$$L^{2}\psi_{+} = j(j+1)\psi_{+} + \kappa\psi_{+} + \frac{1}{4}\psi_{+}$$
  

$$\Rightarrow l_{+}(l_{+}+1) = j(j+1) + \kappa + \frac{1}{4}, \qquad (1.396)$$
  

$$L^{2}\psi_{-} = j(j+1)\psi_{-} - \kappa\psi_{-} + \frac{1}{4}\psi_{-}$$
  

$$\Rightarrow l_{-}(l_{-}+1) = j(j+1) - \kappa + \frac{1}{4}. \qquad (1.397)$$

So, any two-component eigenfunction of  $(\sigma L + 1)$  and  $J^2$  is also an eigenfunction of  $L^2$ . Thus, although the four-component bi-spinor  $\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$  is not an eigenfunction of  $L^2$  (since  $H_D$  does not commute with  $L^2$ )  $\psi_+$  and  $\psi_-$  separately are eigenfunctions of  $L^2$  whose eigenvalues are denoted as  $l_+(l_+ + 1)$  and  $l_-(l_- + 1)$ , respectively. From (1.396)-(1.397) we can read off the relation between  $l_{\pm}$  and  $\pm \kappa$ , namely

$$\psi_{+}: \quad -\kappa = j(j+1) - l_{+}(l_{+}+1) + \frac{1}{4},$$
  
$$\psi_{-}: \quad \kappa = j(j+1) - l_{-}(l_{-}+1) + \frac{1}{4}.$$
 (1.398)

Using, in addition, the fact that  $\kappa = \pm (j + \frac{1}{2})$  we can determine  $l_+$  and  $l_-$  for a given  $\kappa$ . The result is depicted in the table Tab. 1.3.

	$l_+$ $l$	
$\kappa = j + \frac{1}{2}$	$j + \frac{1}{2}$	$j - \frac{1}{2}$
$\kappa = -\left(j + \frac{1}{2}\right)$	$j - \frac{1}{2}$	$j + \frac{1}{2}$

**Table 1.3:** Relation among  $\pm \kappa$  and  $l_+$  and  $l_-$ .

To see how this table is constructed, let us look, e.g., at the first upper entry in the first column, i.e.,  $j + \frac{1}{2}$ . This results from the first equation in (1.398) by writing

$$-\left(j+\frac{1}{2}\right) = j(j+1) - l_{+}(l_{+}+1) + \frac{1}{4}$$

$$= j^{2} + j - l_{+}^{2} - l_{+} + \frac{1}{4}$$

$$\Rightarrow l_{+}^{2} + l_{+} = j^{2} + 2j + \frac{3}{4} = \left(j+\frac{1}{2}\right)^{2} + \left(j+\frac{1}{2}\right). (1.399)$$

This confirms the stated entry in the table. Similarly we would derive another 3 entries in the table Tab. 1.3.

Thus, for given *j* we see that  $l_{\pm}$  can assume two possible values corresponding to two possible values of  $\kappa$ , so instead of  $\kappa$  one can use  $l_{+}$  and  $l_{-}$ . This is particularly convenient since the spectrosopic notation involves orbital angular momentum rather than  $\kappa$  and our results can be better compared with existent spectroscopic data.

After this preliminary we can write  $\psi$  as

$$\psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \begin{pmatrix} g(r)\mathcal{Y}_{j,l_+}^m \\ if(r)\mathcal{Y}_{j,l_-}^m \end{pmatrix}, \qquad (1.400)$$

where  $\mathcal{Y}_{j,l}^m$  stands for a *normalized spin-angular function*, that is the *r*-independent eigenfunction of  $J^2$ ,  $J_z$ ,  $L^2$  and of course  $\hat{\sigma}^2 = (\Sigma/2)^2$  formed by the combination of the Pauli spinor with the *spherical harmonics* of order *l*.

The factorization of the wave function (1.400) is dictated by the same reasoning as in the usual non-relativistic spherical potential problem. Namely, the Hamiltonian  $H_D$  can be for both  $\psi_+$  and  $\psi_-$  formulated directly in terms of  $\hat{\sigma} \cdot L$  and *r*-dependent operator. This, in turn, allows to rewrite the eigenvalue differential equation in terms of two coupled equations for g(r) and f(r). The spin-angular function will get completely factor out from the problem.

In order to understand the structure of  $\mathcal{Y}_{j,l}^m$  let us fisrt recall the Clebsch-Gordan expansion for \*\*\*

Note that  $J_3 = L_3 + \hat{\sigma}_3 \Rightarrow L_3 = m_l = m_j \pm \frac{1}{2}$ .

$$|j, m, l\rangle = a|l; m_l = m_j - \frac{1}{2}\rangle \otimes |\frac{1}{2}; \frac{1}{2}\rangle + b|l; m_l = m_j + \frac{1}{2}\rangle \otimes |\frac{1}{2}; -\frac{1}{2}\rangle,$$
 (1.401)

for any *l*. Here *a* and *b* are Clebsch-Gordan coefficients \*\*\*\* More explicitly, when  $j = l + \frac{1}{2}$ 

$$\mathcal{Y}_{j,l}^{m} = \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}} Y_{l}^{m_{j}-1/2} \begin{pmatrix} 1\\0 \end{pmatrix} + \sqrt{\frac{l-m+\frac{1}{2}}{2l+1}} Y_{l}^{m_{j}+1/2} \begin{pmatrix} 0\\1 \end{pmatrix}, \quad (1.402)$$

and for  $j = l - \frac{1}{2}$ 

$$\mathcal{Y}_{j,l}^{m} = -\sqrt{\frac{l-m+\frac{1}{2}}{2l+1}} \frac{m_{j}-1/2}{l} \begin{pmatrix} 1\\0 \end{pmatrix} + \sqrt{\frac{l+m+\frac{1}{2}}{2l+1}} Y_{l}^{m_{j}+1/2} \begin{pmatrix} 0\\1 \end{pmatrix}. \quad (1.403)$$

We would like to substitute our solution to a Dirac equation and solve it for the radial functions and find the spectrum. In Dirac representation Dirac's equation splits as:

$$H_{D} = \begin{bmatrix} \boldsymbol{\alpha} \cdot \boldsymbol{p} + \beta \boldsymbol{m} + V(r) \end{bmatrix} \Rightarrow H_{D} \Psi = E \Psi \Rightarrow$$

$$\begin{pmatrix} 0 & \boldsymbol{\sigma} \\ \boldsymbol{\sigma} & 0 \end{pmatrix} \begin{pmatrix} \mathbb{I} & 0 \\ 0 & \mathbb{I} \end{pmatrix}$$

$$(\boldsymbol{\sigma} \boldsymbol{p}) \Psi_{-} = (E - V(r) - m) \Psi_{+}$$

$$(\boldsymbol{\sigma} \boldsymbol{p}) \Psi_{+} = (E - V(r) + m) \Psi_{-}$$
(1.404)

Note in this connection that

$$\sigma \cdot \boldsymbol{p} = \underbrace{\frac{(\boldsymbol{\sigma} \cdot \boldsymbol{x})(\boldsymbol{\sigma} \cdot \boldsymbol{x})}{r^{2}}}_{\sigma_{i}\sigma_{j}x_{i}x_{j}=\frac{1}{2}\{\sigma_{i};\sigma_{j}\}x_{i}x_{j}=\boldsymbol{x}^{2}=r^{2}}_{=\frac{(\boldsymbol{\sigma} \cdot \boldsymbol{x})}{r^{2}}\underbrace{(\boldsymbol{\sigma}^{i}\boldsymbol{\sigma}^{j}}_{\delta^{ij}+i\epsilon^{ijk}\boldsymbol{\sigma}^{k}} x^{i}p^{j}) = \frac{(\boldsymbol{\sigma} \cdot \boldsymbol{x})}{r^{2}}(\boldsymbol{x} \cdot \boldsymbol{p}+i\boldsymbol{\sigma} \cdot \boldsymbol{L})$$

$$= \frac{(\boldsymbol{\sigma} \cdot \boldsymbol{x})}{r^{2}}(-ir\frac{\partial}{\partial r}+i\boldsymbol{\sigma} \cdot \boldsymbol{L}) = (\boldsymbol{\sigma} \cdot \hat{\boldsymbol{r}})\left[-i\frac{\partial}{\partial r}+\frac{i\boldsymbol{\sigma} \cdot \boldsymbol{L}}{r}\right]$$
(1.405)

In spherical coord. **x** has radial dir.  $\Rightarrow \mathbf{x} = re_r^s + 0e_\theta^s + 0e_\varphi^s$   $\Delta = e_r^s \frac{\partial}{\partial r} + \frac{1}{r}e_\theta^s \frac{\partial}{\partial \theta} + e_\varphi^s \frac{1}{r\sin\theta} \frac{\partial}{\partial \varphi}$   $\Rightarrow \mathbf{x} \cdot \mathbf{p} = -ir \frac{\partial}{\partial r}$ 

#### Note:

 $\underbrace{\frac{(\sigma \cdot x)}{r}}_{r} \text{ is a pseudoscalar (under parity } x \mapsto -x; r \mapsto r; \sigma \mapsto \sigma)$ 

projection of spin into the unit radius vector

$$\frac{(\boldsymbol{\sigma}\cdot\boldsymbol{x})}{\longrightarrow}\xrightarrow{p}-\frac{(\boldsymbol{\sigma}\cdot\boldsymbol{x})}{\longrightarrow}$$

$$\frac{(\boldsymbol{\sigma} \cdot \boldsymbol{x})}{r} = \boldsymbol{\sigma} \hat{\boldsymbol{r}} = \begin{cases} \hat{r}_x = \sin \theta \cos \varphi \\ \hat{r}_y = \sin \theta \sin \varphi \\ \hat{r}_z = \cos \theta \end{cases} = \begin{pmatrix} \cos \theta & e^{-i\varphi} \sin \theta \\ e^{i\varphi} \sin \theta & -\cos \theta \end{pmatrix}$$

First, the effect of ( $\boldsymbol{\sigma} \cdot \boldsymbol{L}$  on  $J_{jl}^m$  is simple. Namely, observe

$$\underbrace{\hat{K}}_{\beta} = \beta(\Sigma L + 1) = \begin{pmatrix} \sigma L + 1 & 0 \\ 0 & -\sigma L - 1 \end{pmatrix}$$
(1.406)

we already know

$$\Rightarrow \hat{K}\Psi \mapsto -K\Psi \to -K\Psi_{-} = (-\sigma L - 1)\Psi_{-}$$
$$\Rightarrow \sigma L\Psi_{-} = (K - 1)\Psi_{-}$$
and  $-K\Psi_{+} = (\sigma L + 1)\Psi_{+}$ 
$$\Rightarrow \sigma L\Psi_{+} = -(K + 1)\Psi_{+}$$

It is trickier to calculate the effect of the matrix factor

$$\frac{(\boldsymbol{\sigma} \cdot \boldsymbol{x})}{r} = \boldsymbol{\sigma} \hat{\boldsymbol{r}} = \begin{pmatrix} \cos \theta & e^{-i\varphi} \sin \theta \\ e^{i\varphi} \sin \theta & -\cos \theta \end{pmatrix}$$

on the spinor wave functions. In principle, we can carry out the multiplication directly on  $J_{jl}^m$ . Then we would have various identities for spherical harmonics  $Y_l^m(\theta, \varphi)$ .

Note:  $\langle \hat{\pmb{n}} | l, m \rangle = \Psi^m_{\ l}(\theta, \varphi) = \Psi^m_{\ l} | \hat{\pmb{n}} \rangle$ 

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$$\begin{split} |\hat{\boldsymbol{n}}\rangle &= direction \ eigen \ vect. \\ (\langle \boldsymbol{x}|n,l,m\rangle &= R_{ml}(r) \Psi^m_{\ l}(\theta,\varphi)) \end{split}$$

There is an easier way, however. Observe that  $\sigma \hat{r}$  commutes with  $J^2$ ,  $L^2$ ,  $S^2 \left(=\frac{\sigma^2}{4}\right)$  and  $J_3$ .

Proof:

$$[\boldsymbol{\sigma} \cdot \hat{\boldsymbol{r}}; \boldsymbol{J}^2] = \underbrace{[\hat{\boldsymbol{r}} \cdot \boldsymbol{\sigma}; \boldsymbol{L}^2]}_{A} + \underbrace{[\hat{\boldsymbol{r}} \cdot \boldsymbol{\sigma}; \boldsymbol{\sigma}^2/4]}_{B}$$
(1.407)

$$A: \frac{1}{r}\sigma_i[x_i; L^2] = \frac{\sigma_i}{r}L_j\underbrace{[x_i; L_j]}_{-i\epsilon_{jik}x_k} + \frac{\sigma_i}{r}\underbrace{[x_i; L_j]}_{-i\epsilon_{jik}x_k}L_j$$
$$= \frac{\sigma_i}{r}[-i\underbrace{\epsilon_{jik}}_{antisym}\underbrace{(L_jx_k + x_kL_j)}_{sym}] = 0$$

$$B : [\hat{r} \cdot \sigma; \sigma^2/4] = \frac{\hat{r}_i}{4} \{ [\sigma_i; \sigma_j] \sigma_j + \sigma_j [\sigma_i; \sigma_j] \}$$
$$= \frac{\hat{r}_i}{4} \{ 2i\epsilon_{ijk}\sigma_k\sigma_j + \sigma_j 2i\epsilon_{ijk}\sigma_k \}$$
$$= \frac{\hat{r}_i}{4} 2i \underbrace{\epsilon_{ijk}}_{\text{antisym.}} \underbrace{\{\sigma_k\sigma_j + \sigma_j\sigma_k\}}_{\text{sym.}} = 0$$

$$[\boldsymbol{\sigma} \cdot \hat{\boldsymbol{r}}; J_3] = \underbrace{[\boldsymbol{\sigma} \cdot \hat{\boldsymbol{r}}; L_3]}_{C} + \underbrace{[\hat{\boldsymbol{r}} \cdot \boldsymbol{\sigma}; \boldsymbol{\sigma}_3/2]}_{D}$$
(1.408)

$$C: \frac{\sigma_i}{r} \underbrace{[x_i; L_3]}_{-i\epsilon_{3ij}x_i} = -i\epsilon_{3ij}\sigma_i \hat{r}_j$$

$$D: \frac{\hat{r}_i}{2} \underbrace{[\sigma_i; \sigma_j]}_{2i\epsilon_{i3k}\sigma_k} = i\epsilon_{i3k}\hat{r}_i\sigma_k = -i\epsilon_{3ik}\hat{r}_i\sigma_k = i\epsilon_{3jk}\sigma_j\hat{r}_k$$

So  $\sigma \hat{r}$  is simultaneously diagonal with  $J^2$ ,  $J_3$ . Since  $(\sigma \hat{r})^2 = 1$ , its eigenvalues are ±1.

Since  $\sigma$   $\hat{r}$  is a pseudo-scalar under rotation, if we evaluate its pseudo-vectorvector

effect at one particular  $\hat{r}$  (say  $\hat{z}$ ), it should behave that way for all  $\hat{r}$ .  $\hat{z}$  corresponds to  $\theta = 0 \Rightarrow$ 

$$\underbrace{Y_l^m(\theta=0,\varphi)=\sqrt{\frac{2l+1}{4\pi}}\delta_{m,0}}_{\text{see, e.g. Grandshteyn-Ryzhik}}$$

In which case

$$Y_{j=l\pm 1/2;l}^{m_j} = \frac{1}{\sqrt{2l+1}} \begin{bmatrix} \pm \sqrt{l\pm m+1/2} & Y_l^{m_j-1/2} \\ \sqrt{l\mp m+1/2} & Y_l^{m_j+1/2} \end{bmatrix} = \frac{1}{\sqrt{4\pi}} \begin{bmatrix} \pm \sqrt{l\pm m+1/2} & \delta_{m;1/2} \\ \sqrt{l\mp m+1/2} & \delta_{m;-1/2} \end{bmatrix}$$

or

$$J_{j;l=j\mp 1/2}^{m_j}(\theta=0;\varphi) = \sqrt{\frac{j+1/2}{4\pi}} \begin{bmatrix} \pm \delta_{m;1/2} \\ \delta_{m;-1/2} \end{bmatrix}$$

 $\Rightarrow$ 

$$\begin{split} \sigma \cdot \hat{z} \ J_{j;l=j\mp 1/2}^{m}(\theta = 0;\varphi) &= \sqrt{\frac{j+1/2}{4\pi}} \begin{bmatrix} \pm \delta_{m;1/2} \\ -\delta_{m;-1/2} \end{bmatrix} \\ &= -\sqrt{\frac{j+1/2}{4\pi}} \begin{bmatrix} \mp \delta_{m;1/2} \\ \delta_{m;-1/2} \end{bmatrix} = -Y_{j;l=j\pm 1/2}^{m}(\theta = 0;\varphi) \end{split}$$

or by rotating both sides of the equation to general  $\hat{r}$ 

$$\Rightarrow (\boldsymbol{\sigma} \cdot \hat{\boldsymbol{r}}) J_{j;l=j \neq 1/2}^{m}(\theta; \varphi) = -Y_{j;l=j \pm 1/2}^{m}(\theta; \varphi)$$
(1.409)

Thus

$$\begin{split} (\boldsymbol{\sigma}\boldsymbol{r})\Psi_{-} &= \frac{i(\boldsymbol{\sigma}\boldsymbol{x})}{r} \left( -i\frac{\partial}{\partial r}f + \frac{i(k-1)}{r}f \right) J_{j,l_{-}}^{m} \\ &= \frac{\boldsymbol{\sigma}\boldsymbol{x}}{r} J_{j,l_{-}}^{m} \left( \frac{\partial f}{\partial r} - \frac{(k-1)}{r}f \right) \\ &= -\frac{\partial f}{\partial r} J_{j,l_{+}}^{m} - \frac{(1-k)}{r} f J_{j,l_{-}}^{m} \end{split}$$

similarly

$$(\sigma r)\Psi_{+} = \frac{(\sigma x)}{r} \left( -i\frac{\partial}{\partial r} + i\sigma L \right) g J_{j,l_{+}}^{m}$$
$$= \frac{\sigma x}{r} J_{j,l_{+}}^{m} \left( -i\frac{\partial g}{\partial r} - i\frac{(k+1)}{r}g \right)$$
$$= i\frac{\partial g}{\partial r} J_{j,l_{-}}^{m} + i\frac{(k+1)}{r}g J_{j,l_{+}}^{m}$$

Note: The spin-angular functions completely drop out.

By pluging to decoupled Dirac equation we get

$$-\frac{\mathrm{d}f}{\mathrm{d}r} - \frac{(1-k)}{r}f = (E-V-m)g \quad (\bullet)$$

$$-\frac{\mathrm{d}g}{\mathrm{d}r} + \frac{(k+1)}{r}g = (E - V + m)f \quad (\bullet \bullet)$$

As in non-relativistic QM we introduce the ansatzes

$$F(r) = rf(r);$$
  $G(r) = rg(r)$ 

are supposed to be non-singular  $\rightarrow f(r)$ ;  $g(r) \sim \frac{1}{r}$ , r <<1

$$\Rightarrow \frac{\mathrm{d}F(r)}{\mathrm{d}r} = f(r) + r\frac{\mathrm{d}f}{\mathrm{d}r} \Rightarrow \frac{\mathrm{d}f}{\mathrm{d}r} + \frac{f}{r} = \frac{1}{r}\frac{\mathrm{d}F(r)}{\mathrm{d}r}$$

$$\Rightarrow \frac{\mathrm{d}g}{\mathrm{d}r} + \frac{g}{r} = \frac{1}{r}\frac{\mathrm{d}G}{\mathrm{d}r}$$

$$\begin{aligned} (\bullet) & \Rightarrow \ -\frac{1}{r}\frac{\mathrm{d}F}{\mathrm{d}r} + \frac{kF}{r^2} = (E - V - m)G/r \quad /(\cdot(-r)) \\ & \Rightarrow \ \frac{\mathrm{d}F}{\mathrm{d}r} + \frac{k}{r}F = -(E - V - m)G \end{aligned}$$

$$(\bullet \bullet) \implies -\frac{1}{r}\frac{\mathrm{d}G}{\mathrm{d}r} + \frac{kG}{r^2} = (E - V + m)F/r \quad /(\cdot r)$$
$$\implies \frac{\mathrm{d}G}{\mathrm{d}r} + \frac{k}{r}G = (E - V + m)F$$

- anomalous Zeeman ef.

- free spherical waves

- exact solution to the Coulomb scattering problem

- etc.

With this system of equations a variety of problems can be attacked. We shall consider only one problem, i.f. electron bound to the atomic nucleus by a Coulomb potential. This problem can be solved exactly.

Consider 
$$V(r) = -\frac{Ze^2}{r}$$
, where  $e = \frac{e}{\sqrt{4\pi\epsilon_0}}$ .

Solution: Let us first look at the asymptotic behavior of *F* and *G* at  $r \to \infty$ 

$$\frac{\mathrm{d}G}{\mathrm{d}r} = (E+m)F; \quad \frac{\mathrm{d}F}{\mathrm{d}r} = -(E-m)G$$

$$\frac{d^2G}{dr^2} = -(E^2 - m^2)G$$
 and  $\frac{d^2F}{dr^2} = -(E^2 - m^2)F$ 

$$\Rightarrow G; F \sim e^{-\sqrt{m^2 - p \mathcal{E}_{si}^2} t_{ive}}$$

for  $r \rightarrow 0$ 

$$\frac{kG}{r} = -rF$$
 and  $\frac{-kF}{r} = rG$ 

$$\Rightarrow kG = 2e^2F$$
 and  $kF = 2e^2G$ 

 $\Rightarrow$  *G* and *F* have the same asymptotic at  $r \rightarrow 0$ , due to regularity *G*, *F*  $\propto r^{s>0}$ 

To work with dimensionless quantities we can introduce the following scaled variables

 $\alpha_1 = (m + E), \ \alpha_2 = (m - E), \ \gamma = Z\hat{e}^2 = Z \underline{\alpha} \simeq Z/137, \ \rho = \sqrt{\alpha_1 \alpha_2}r$ fine structure constant

So, the coupled equations  $(\bullet)$  and  $(\bullet \bullet)$  get a form

$$(\bullet) \Rightarrow \left(\frac{\mathrm{d}}{\mathrm{d}r} - \frac{k}{r}\right) F - \left[-(E - m) - \frac{\gamma}{r}\right] G = 0 \quad /\cdot \frac{1}{\sqrt{\alpha_1 \alpha_2}} \\ \Rightarrow \left(\frac{\mathrm{d}}{\mathrm{d}\rho} - \frac{k}{\rho}\right) F - \left[\sqrt{\frac{\alpha_2}{\alpha_1}} - \frac{\gamma}{\rho}\right] G = 0$$

similarly

$$\Rightarrow \left(\frac{\mathrm{d}}{\mathrm{d}\rho} - \frac{k}{\rho}\right)G - \left[\sqrt{\frac{\alpha_1}{\alpha_2}} + \frac{\gamma}{\rho}\right]F = 0$$

As in the non-relativistic treatment of the hydrogen atom, we seek solutions in this form

$$F = \underbrace{e^{-\rho}}_{r \to \infty} \underbrace{\rho^s}_{r \to 0} \sum_{m=0}^{r} a_m \rho^m; \quad G = e^{-\rho} \rho^s \sum_{m=0}^{r} b_m \rho^m$$

"s" furthere constrained normalization condition for  $\Psi$ 

 $E = E_{kin.} + E_{pot.} + m$ classically  $E_{kin.} + E_{pot.} = const$  for all p, so if  $p = 0 \Rightarrow const$  is negativ  $\Rightarrow E - m < 0 \Rightarrow E^2 - m^2 < 0$ or  $m^2 - E^2 > 0$  Substituting this to  $(\bullet)$  and  $(\bullet \bullet)$  we get recursion treat on

$$\left(\frac{\mathrm{d}}{\mathrm{d}\rho}F = -F + e^{-\rho}\sum_{m=0}a_m(m+s)\rho^{m+s-1}\right)$$

$$(\bullet) \Rightarrow -e^{-\rho} \sum_{m=0}^{\infty} a_m \rho^{m+s} + e^{-\rho} \sum_{m=0}^{\infty} a_m (m+s) \rho^{m+s-1} - k e^{-\rho} \sum_{m=0}^{\infty} a_m \rho^{m+s-1} -e^{-\rho} \sum_{m=0}^{\infty} \left( b_m \sqrt{\frac{\alpha_2}{\alpha_1}} \right) \rho^{m+s} + e^{-\rho} \sum_{m=0}^{\infty} b_m \gamma \rho^{m+s-1} = 0$$

comparin coefficients at  $\rho^{s+m-1}$ 

for  $m \neq 0$  ( $a \ge 1$ )

$$a_m(m+s-k) - a_{m-1} + \gamma b_m - \sqrt{\frac{\alpha_2}{\alpha_1}} b_{m+1} = 0$$
 (1.410)

similarly

$$(\bullet) \Rightarrow b_m(m+s+k) - b_{m-1} + \gamma a_m - \sqrt{\frac{\alpha_1}{\alpha_2}} a_{m-1} = 0$$
 (1.411)

for m = 0

$$(\bullet) \Rightarrow a_0(s-k) + \gamma b_0 = 0$$

$$(\bullet \bullet) \Rightarrow b_0(s+k) - \gamma a_0 = 0$$

which in matrix notation reads as

$$\begin{pmatrix} s-k & \gamma \\ -\gamma & s+k \end{pmatrix} \begin{pmatrix} a_0 \\ b_0 \end{pmatrix} = 0.$$
 (1.412)

Since  $a_0$  and  $b_0$  must have non-trivial solution we require that

$$\begin{vmatrix} s-k & \gamma \\ -\gamma & s+k \end{vmatrix} = 0.$$
(1.413)

This implies that  $s^2 - k^2 + \gamma^2 = 0$  or equivalently  $s = \pm \sqrt{k^2 - \gamma^2}$ .

Note:

There is an important restriction on the scaling exponent "s" from

the normalizability of Dirac's wave function.

$$\begin{split} \|\Psi\|^{2} &= \int \overline{\Psi} \gamma^{0} \Psi = \int \Psi^{+} \Psi < \infty \\ &= \int d\Omega dr r^{2} \begin{pmatrix} gJ \\ ifJ \end{pmatrix}^{+} \begin{pmatrix} gJ \\ ifJ \end{pmatrix} \\ &= \int \underbrace{|g|^{2} r^{2} dr}_{|G|^{2}} \int \underbrace{|J|^{2} d\Omega}_{<\infty} + \int \underbrace{|f|^{2} r^{2} dr}_{|F|^{2}} \int \underbrace{|J|^{2} d\Omega}_{<\infty} < \infty (\text{required}) \end{split}$$

$$\Rightarrow \int |G|^2 \mathrm{d}r < 0; \ \int |F|^2 \mathrm{d}r < 0 \iff \int |G|^2 \mathrm{d}\rho < 0; \ \int |F|^2 \mathrm{d}\rho < 0$$

 $\Rightarrow$  *F* and *G* must behave better than  $\rho^{-1/2}$  (e.g.  $\rho^{-1/2+\epsilon(>0)}$ ) at the origin  $\Rightarrow s > -1/2$ 

However, since

$$k^2 - \gamma^2 \ge \min(k^2) - \gamma^2 \simeq 1 - Z^2 \alpha^2 \Longrightarrow k^2 - \gamma^2 \ge 1 - Z^2 \alpha^2$$

Now

$$-\frac{1}{2} < s = \pm \sqrt{k^2 - \gamma^2}$$

$$1)\frac{1}{2} > \sqrt{k^2 - \gamma^2} \ge \sqrt{1 - Z^2 \alpha^2} \in (0, 99..., 0, 64...) \text{ (typical } Z < 105)$$

$$2)\frac{1}{2} > -\sqrt{k^2 - \gamma^2}$$
1) cannot be solved, 2) is OK

Back to recurence equations.

We know that F and G must be normalizable well behaved functions, so particularly for large m we have

$$(\bullet) \Rightarrow ma_m - a_{m-1} + \gamma b_m - \frac{\alpha_2}{\alpha_1} b_{m-1} = 0$$
  
$$(\bullet \bullet) \Rightarrow mb_m - b_{m-1} - \gamma a_m - \frac{\alpha_1}{\alpha_2} a_{m-1} = 0 / \cdot \sqrt{\frac{\alpha_2}{\alpha_1}} \text{ and subtract}$$
  
$$\Rightarrow \left(m + \gamma \sqrt{\frac{\alpha_2}{\alpha_1}}\right) a_m + \left(\gamma - m \sqrt{\frac{\alpha_2}{\alpha_1}}\right) b_m = 0 / \cdot \sqrt{\alpha_1}$$
  
$$\Rightarrow (\sqrt{\alpha_1}m + \gamma \sqrt{\alpha_2}) a_m + (\sqrt{\alpha_1}\gamma - m \sqrt{\alpha_2}) b_m = 0$$
  
$$\Rightarrow a_m = \frac{(m\sqrt{\alpha_2} - \gamma \sqrt{\alpha_1})}{(m\sqrt{\alpha_1} + \gamma \sqrt{\alpha_2})} b_m$$

Plugging this to  $(\bullet \bullet)$  we get

k = (j + 1/2) =positive (j = 1/2; 3/2; 5/2..) $\min(k^2) = 1$ 

$$\begin{split} mb_m - b_{m-1} &- \gamma \frac{(m\sqrt{\alpha_2} - \gamma\sqrt{\alpha_1})}{(m\sqrt{\alpha_1} + \gamma\sqrt{\alpha_2})} b_m - \sqrt{\frac{\alpha_1}{\alpha_2}} \left( \frac{(m-1)\sqrt{\alpha_2} - \gamma\sqrt{\alpha_1}}{(m-1)\sqrt{\alpha_1} + \gamma\sqrt{\alpha_2}} \right) b_{m-1} = 0\\ \Rightarrow b_m \left[ m - \gamma \frac{(m\sqrt{\alpha_2} - \gamma\sqrt{\alpha_1})}{(m\sqrt{\alpha_1} + \gamma\sqrt{\alpha_2})} \right] - b_{m-1} \left[ 1 + \frac{(m-1)\sqrt{\alpha_2} - \gamma\sqrt{\alpha_1}}{(m-1)\sqrt{\alpha_1} + \gamma\sqrt{\alpha_2}} \right] = 0 \end{split}$$

For large *m* (large summation order) we have

$$b_m \left[ m - \gamma \sqrt{\frac{\alpha_2}{\alpha_1}} \right] - b_{m-1} [1+1] = 0$$
  

$$\Rightarrow b_m = \frac{2}{m - \gamma} \underbrace{\sqrt{\frac{\alpha_2}{\alpha_1}}}_{Const.} b_{m-1} \sim \frac{2}{m} b_{m-1}$$

for large *m* 

$$a_m \sim b_m \sqrt{\frac{\alpha_2}{\alpha_1}}$$
  

$$\Rightarrow \text{ since } \frac{b_m}{b_{m-1}} = \frac{2}{m} \Rightarrow \frac{a_m}{a_{m-1}} = \frac{2}{m}$$
  

$$\Rightarrow \sum_{m=0}^{\infty} a_m \rho^m \sim \sum_{m=0}^{\infty} \frac{1}{m!} (2\rho)^m \sim e^{2\rho}$$
  

$$\Rightarrow \sum_{m=0}^{\infty} b_m \rho^m \sim e^{2\rho}$$

 $\Rightarrow$  if  $\sum_{n=0}$  is infinite  $\Rightarrow$   $F \sim e^{\rho}$ ,  $G \sim e^{\rho} \Rightarrow$  diverges at  $r \rightarrow \infty$  (if wave functions are nor normalizable)

$$\Rightarrow \exists n_c \text{ s. t. for } \forall n > n_c, a_n; b_n = 0$$
  
We know that  $a_m = \sqrt{\frac{\alpha_2}{\alpha_1}} b_m$ , assume that

$$n_c = m - 1 \Longrightarrow a_{n_c} = -\sqrt{\frac{\alpha_2}{\alpha_1}} b_{n_c} \tag{1.414}$$

(both series terminate at the same  $n_c$ )

Now we know the ratio  $\frac{a_{n_c}}{b_{n_c}}$ , so no we are in position to use the recurrence equations to find on (??), (??) to find relations between  $b_{n_c}$  and  $a_{n_c}$  (whose ratio we know). From this we get equation for *E* (since *E* is in  $\alpha_1$  and  $\alpha_2$ ).

Let us multiply the first recursion relation by  $\alpha_1$  and the second by  $\sqrt{\alpha_1 \alpha_2}$ , set  $m = n_c$  and subtract, i.e.

$$(*) \alpha_1(s + n_c - k)a_{n_c} - \alpha_1 a_{n_c} - \alpha_1 a_{n_c-1} + \alpha_1 \gamma b_{n_c} - \sqrt{\alpha_1 \alpha_2} b_{n_c-1} = 0$$

$$(**) \sqrt{\alpha_1 \alpha_2}(s + n_c + k)b_{n_c} - \sqrt{\alpha_1 \alpha_2} a_{n_c} - \sqrt{\alpha_1 \alpha_2} \gamma a_{n_c} - \alpha_1 a_{n_c-1} = 0$$

$$(*) - (**) \Rightarrow$$

$$\begin{split} &\alpha_1(s+n_c-k)a_{n_c}+\sqrt{\alpha_1\alpha_2}\gamma a_{n_c}=\sqrt{\alpha_1\alpha_2}(s+n_c+k)b_{n_c}-\alpha_1\gamma b_{n_c}\\ \Leftrightarrow &a_{n_c}[\alpha_1(s+n_c-k)+\sqrt{\alpha_1\alpha_2}\gamma]=b_{n_c}[\sqrt{\alpha_1\alpha_2}(s+n_c+k-\alpha_1\gamma)]\\ &[\alpha_1(s+n_c-k)+\sqrt{\alpha_1\alpha_2}\gamma]=\underbrace{[\sqrt{\alpha_1\alpha_2}(s+n_c+k)-\alpha_1\gamma]}_{-[\alpha_1(s+n_c+k)-\alpha_1\sqrt{\frac{\alpha_1}{\alpha_2}}\gamma)}\left(-\sqrt{\frac{\alpha_1}{\alpha_2}}\right)\\ &2\alpha_1(s+n_c)=\gamma\left(\alpha_1\sqrt{\frac{\alpha_1}{\alpha_2}}-\sqrt{\alpha_1\alpha_2}\right)/\cdot\sqrt{\frac{\alpha_2}{\alpha_1}}\\ &2\sqrt{\alpha_1\alpha_2}(s+n_c)=\gamma(\alpha_1-\alpha_2)\\ &2\sqrt{m^2-E^2}(s+n^c)=\gamma[m+E-(m-E)]=2\gamma E\\ \Rightarrow\sqrt{m^2-E^2}(s+n_c)=E\gamma = \text{quadratic eq.} \end{split}$$

which implies that

$$E = \frac{m}{\sqrt{1 + \frac{\gamma^2}{(s+n_c)^2}}} = \frac{m}{\sqrt{1 + \frac{Z^2 \alpha^2}{(n_c \sqrt{k^2 - \gamma^2})^2}}}$$
  
=  $\frac{m}{\sqrt{1 + \frac{Z^2 \alpha^2}{(n_c \sqrt{(j+1/2)^2 - Z^2 \alpha^2})^2}}}$ . (1.415) negative energies are occupied  
 $\alpha = \hat{e}^2 = \frac{e^2}{4\pi\epsilon_0} = \frac{1}{137}$ 

Note that *E* depends only on  $n_c$  and j + 1/2 = |k|. In order to compare (1.415) with the corresponding expression obtained in the Schrödinger theory, we define  $n \equiv n_c + (j + 1/2) = n_c + |k|$ .

we know it is integer

Since the minimum value of  $n_c = 0$ , we have

$$0 \le n_c = n - (j + 1/2) \implies n \ge (j + 1/2) = |k|, \qquad (1.416)$$

which is at least unity. Expanding (1.415) we get

$$E = m \left[ 1 - \frac{1}{2} \frac{(Z\alpha)^2}{n^2} - \frac{1}{2} \frac{(Z\alpha)^4}{n^3} \underbrace{\left( \frac{1}{j+1/2} - \frac{3}{4n} - \cdots \right)}_{>0} \right], \quad (1.417)$$

since

$$\frac{1}{2}\alpha^2 mc^2 = \left\{ \hat{e}^2 = \alpha = \frac{e^2}{4\pi\epsilon_0} \right\} = \frac{1}{2}m \frac{e^4}{(4\pi\epsilon_0)^2} = \frac{e^4m}{32\pi^2\epsilon_0^2} = \frac{e^2}{8\pi a_B} , (1.418)$$

where  $a_B = 4\pi\epsilon_0/(m_e e^2) = 1/(m_e \alpha)$  is *Bohr's radius*. We see that "*n*" is indeed identical with the familiar "principal quantum number" of non-rel. QM.

Note:

A catastrophe occures in the original formula for *E* when Z = 137 $\Rightarrow \sqrt{(j+1/2) - Z^2 \alpha^2}$  becomes imaginar.  $j = n - n_c - 1/2$ max J = n - min(n<sub>c</sub>) - 1/2 = n - 1/2 n = 1,2,..; j = 1/2,3/2,... Note:

First dominant contribution comes from

$$-\frac{1}{2}\frac{mc^{2}(Z\alpha)^{2}}{n^{2}} = \left\{\alpha = \frac{e^{2}}{4\pi\epsilon_{0}\hbar c}\right\} = -\frac{1}{2}\frac{mc^{2}Z^{2}e^{4}}{n^{2}(4\pi\epsilon_{0}\hbar c)^{2}} = -\frac{Z^{2}}{2n^{2}}\frac{e^{2}}{4\pi}\underbrace{\frac{e^{2}m}{4\pi\epsilon_{0}\hbar^{2}}}_{\frac{1}{a_{B}}} = -\frac{Z^{2}e^{2}}{8^{2}a_{B}}$$

 $\Rightarrow$  Higher order corrections are due to spin and relativity removes the energy degeneracy in an observable way.

For a give *n*, higher *j*-states are at higher energy levels.

In the Dirac theory each state of a hydrogen atom can be completely characterized by  $n_c$  (or n),  $\kappa_{I \text{ and } J}$  and  $j_3$  (only on the level of statevec-

tors).

One can translate this classification scheme into the more familiar spectroscopic notation.

It should be stressed that even though  $L^2$  is not "good" in the relativistic theory, it is customary to use the notation

 $nx_j$ 

*n* - principal quantum number n = 1, 2, ...

*x* - orbital quantum number  $l_{+} = (0, 1, 2, ...) = (s, p, d, ...)$ 

*j* - total angular momenta j = 1/2; 3/2; 5/2; ...

$$\begin{aligned} \kappa &= j + 1/2 & j + 1/2 \\ \kappa &= -(j + 1/2) & j - 1/2 \end{aligned}$$

e. g. 2*p*<sub>1/2</sub>

#### Note:

The orbital angular momentum  $l_+$  of the upper two-component wave function (in non-rel. case will correspond to Schrödinger-Pauli theory) determines the orbital angular momentum in the spectroscopic language.

Fine structure of the spectrum is a new phenomenon w.r.t. s.e. It is the difference between energy levels of different *j* but identical *n*.

 $a_B$  - most probable distance of electrons from nucleus in its ground state

Table 1.4

$$\begin{split} n &= n_c + j + 1/2 \Rightarrow n - j - 1/2 \geqslant 0 \\ \Rightarrow j - 1/2 \\ \max J &= l_+ + 1/2 \leqslant n - 1/2 \\ \Rightarrow l_+ \leqslant n - 1 \end{split}$$

n	$n_c = n -  \kappa  \ge 0$	$\kappa = \pm (j + 1/2)$	spectroscopic notation	Table 1.5
1	0	$-1  j = 1/2; \ l_+ = 0$	$1s_{1/2}$	
2	1	-1 $j = 1/2; l_+ = 0$	$2s_{1/2}$	
2	1	1 $j = 1/2; l_+ = 1$	$2p_{1/2}$	
2	0	-2 $j = 3/2; l_+ = 1$	$2p_{3/2}$	
3	2	-1 $j = 1/2; l_+ = 0$	$3s_{1/2}$	
3	2	1 $j = 1/2; l_+ = 1$	$3p_{1/2}$	
3	1	-2 $j = 3/2; l_+ = 1$	$3p_{3/2}$	
3	1	2 $j = 3/2; l_+ = 2$	$3d_{3/2}$	
3	0	$  -3  j = 5/2; \ l_+ = 2$	$3d_{5/2}$	



nonrelativistic Dirac equation Lamb shift hyperfine structure



## 1.16 Relativistic higher-spin wave equations

Apart from Klein-Gordon wave equation (for spin - 0 particle) and Dirac's wave equation (for spin -1/2 particle), there exists a number of relativistic higher-spin wave equations.

#### **Examples of higher-spin wave equations:**

▶ "Maxwell equation" (for *massless* spin - 1 particle)

 $\partial_{\mu}\partial^{\mu}A^{\nu} = e\overline{\psi}\gamma^{\nu}\psi$  (valid in Lorentz gauge where  $\partial_{\mu}A^{\mu} = 0$ )

This wave equation describes a photon in interaction with electrically charges spin 1/2 particle. For completeness, this equation should be complemented also with corresponding Dirac's equation with electromagnetic potential included (e.g., via minimal substitution). Note that the role of wave function for a photon is played by the gauge potential (i.e., wave function carries a vector index as an index of internal symmetry,

**Figure 1.7:** Schematic energy level diagram for *H* atom with relativistic corrections included.

Recall that the intensity of electromagnetic radiation (i.e., square of its amplitude — be it *E* or *B*) is due to Einstein's explanation of the *photoelectric effect* proportional to the (average) density of photons in the radiation. In particular, if the intensity of monochromatic electromagnetic field is sufficiently low so that it can support only *one* quantum of energy — photon, then the corresponding field can be interpreted as being proportional to *probability density amplitude*.

Note that

 $\sum_{i=1}^{3} S_{i}^{2} \; = \; s(s+1) \mathbbm{1}_{3\times 3} \; = \; 2 \cdot \mathbbm{1}_{3\times 3} \; ,$ 

which implies that *S* indeed describes a particle with spin s = 1.

which in turn means that it transforms in the vector representation of Lorentz group).

Single photon equation without any source term is described by the conventional system of Maxwell equations. In this connection it is interesting to observe that Maxwell equations can be equivalently written as

$$\begin{aligned} i \frac{\partial E}{\partial t} &= \frac{1}{i} S \cdot \boldsymbol{\nabla}(iB) \,, \\ i \frac{\partial iB}{\partial t} &= \frac{1}{i} S \cdot \boldsymbol{\nabla}(E) \,, \end{aligned}$$

where  $(S_i)_{jk} = -i\varepsilon_{ijk}$  represents angular momentum generator in *adjoint representation* (recall that  $[S_i, S_j] = i\varepsilon_{ijk}S_k$ ).

This system of equations should be compared to the system of equations for massless spin 1/2 particle (so called *Weyl equations*)

$$\begin{split} &i\frac{\partial\varphi}{\partial t} &=& \frac{1}{i}\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}(\boldsymbol{\chi})\,,\\ &i\frac{\partial\chi}{\partial t} &=& \frac{1}{i}\boldsymbol{\sigma}\cdot\boldsymbol{\nabla}(\boldsymbol{\varphi})\,. \end{split}$$

Here Dirac's bispinor

$$\psi = \left(\begin{array}{c} \varphi \\ \chi \end{array}\right).$$

So, we see that matrices  $S_i$  play for photon (i.e., particle with spin s = 1 and rest mass  $m_0 = 0$ ) the same role as Pauli matrices for spin 1/2 massless particles (so called Weyl fermions). Similarly, (E, iB) is analogous to  $(\varphi, \chi)$ .

► *Proca equation* (for *massive* spin - 1 particle)

$$\partial_{\mu}(\partial^{\mu}A^{\nu} - \partial^{\nu}A^{\mu}) + mA^{\nu} = 0.$$

This wave equation can be, in principle, used to describe such particles as, e.g.,  $W^{\pm}$  or  $Z^{0}$  bosons.

► *Rarita–Schwinger equation* (for massive spin - 3/2 particle)

$$\left(\epsilon^{\mu\nu\rho\sigma}\gamma^5\gamma_\nu\partial_\rho + m\sigma^{\mu\sigma}\right)\psi_\sigma = 0,$$

where  $\sigma^{\mu\nu} = (i/2)[\gamma^{\mu}, \gamma^{\nu}]$  is a Lorentz group generator in bispinor representation. This wave equation can be, in principle, used to describe *gravitino* that is predicted in supersymmetric theories (SUSY).

- ► *Bargmann-Wigner equation* (for massive arbitrary spin free particle)
  - quite complicated system of equations

Relativistic wave equations have a number of conceptual difficulties.

- ► No simple way to include multi-particle interactions.
- Strictly single-particle description does not allows (is not applicable for) unstable particles or resonances.
- Various paradoxes: "Zitterbewegung", Klein's paradox, problematic probabilistic interpretations (we already seen for Klein-Gordon particle).
- Single-particle picture is not tenable beyond energies that allow for pair (or multi-particle) production.
- No elementary particles has been observed beyond spin 1 particles, though there are various theoretical reasons supporting existence of higher spin particles, e.g., SUSY predicts 3/2-spin particle — gravitino, and quantum gravity predicts spin 2 particle — graviton.

These arguments provide good reasons for abandoning relativistic wave equations — higher-spin wave equations in particular. On the other hand, lower-spin wave equations (such as those with spin 0, 1/2 and 1) are often used as a starting point in setting up corresponding Quantum Field Theories via the so-called *second quantization procedure* (see following chapter).

# Quantum Field Theory I

## 2.1 Why Quantum Field Theory?

Let us now put forward a couple of reasons that explain a conceptual inevitability of quantum field theory.

**I.** — The combination of quantum mechanics and special relativity implies that particle number is not conserved. Relativity necessarily brings in the possibility of conversion of mass into energy and vice versa, i.e., the creation and annihilation of particles. For instance,  $\beta$  decay of the neutron via  $n \rightarrow p + e^- + \bar{v}_e$  or positron-electron annihilation  $e^+e^- \rightarrow 2\gamma$ . There are also situations when the number of particles of given species is not conserved, even though the number of particles of all types taken together is conserved.



**Figure 2.1:** Here we show an extreme demonstration of particle creation. This comes from the Relativistic Heavy Ion Collider (RHIC) at Brookhaven, Long Island. This machine crashes gold nuclei together, each containing 197 nucleons. The resulting explosion contains up to 10,000 particles, captured here in all their beauty by the STAR detector.

It should be stressed that the creation of particles is impossible to avoid whenever one tries to locate a particle of mass *m* within its Compton wavelength. Indeed, from Heisenberg's uncertainty relation we find that (consider motion along *x* direction)

$$\begin{aligned} \sigma_E^2 \sigma_x^2 &\geq \frac{1}{4} \left| \langle [\hat{H}, x] \rangle_{\psi} \right|^2 &= \frac{1}{4} \left| \left\langle [\sqrt{p_x^2 c^2 + m^2 c^4}, x] \right\rangle_{\psi} \right|^2 \\ &= \frac{\hbar^2}{4} \left| \left\langle p_x c^2 / \sqrt{p_x^2 c^2 + m^2 c^4} \right\rangle_{\psi} \right|^2 \\ &= \frac{\hbar^2}{4} \left| c + O\left( \left\langle \frac{m^2 c^4}{p_x^2 c^2} \right\rangle_{\psi} \right) c \right|^2 \sim \frac{\hbar^2 c^2}{4} . \end{aligned}$$
(2.1)

This implies that  $\sigma_E \sigma_x = \Delta E \Delta x \sim \hbar c/2$ . If we assume that  $\Delta x \sim \lambda_C = \hbar/mc$ , then we have  $\Delta E \sim mc^2$ . Therefore, in a relativistic theory, the fluctuations of the energy are enough to allow the creation of particles out of the vacuum. In the case of spin  $\frac{1}{2}$  particle, the Dirac sea picture shows clearly how, when the energy fluctuations are of order  $mc^2$ , electrons from the Dirac sea can be excited to positive energy states, thus creating electron-positron pairs. So, at distances shorter than

particle's Compton wavelength there is a high probability that we will see particles swarming around the original particle we put in.

#### Note about Compton wavelength

Particle's (reduced) Compton wavelength  $\lambda_C = \hbar/mc$  is always smaller than the corresponding de Broglie wavelength  $\lambda_{dB} = \hbar/|\mathbf{p}|$ . In fact, we can say that:

- $\lambda_{dB}$  is the distance at which the wave nature of a particle is apparent
- ► *λ<sub>C</sub>* is the distance at which the concept of a single particle breaks

In order to discuss such processes, the usual formalism of many-body quantum mechanics with wave functions of fixed number of particles, has to be augmented by including the possibility of creation and annihilation of particles via interaction.

**II.** — Ordinary (non-relativistic) point-particle QM can deal with the quantum description of a many-body system in terms of many body wave functions. This is important, e.g., in atomic, molecular or condense matter physics. Similar generalization for relativistic particles would be desirable. Problem with this generalization, however, starts already at classical level. There does not exist any generalization to a relativistically invariant interacting many-body theory — not even for 2 interacting particles. This is known as *Leutwyler's no-interaction theorem* 

Any *finite number* of point particles cannot interact in such a way that the principles of special relativity are respected, i.e. that the system provides a representation of the Lorentz (or more generally Poincare) algebra. Accordingly, classical relativistic point particles are necessarily free, as a consequence of Poincare invariance.

#### Note

The only exception are two particles in one spatial dimension confined to each other by a linearly rising potential.

In contrast to point particles, strings (i.e., 1 dimensional objects) can interact relativistically in higher dimensions, without violating Leutwyler's non-interaction theorem.

Hence, it is not surprising that particle physics is based on Quantum Field Theory (i.e., infinite number of degrees of freedom) rather than on relativistic point particle quantum mechanics.

**III.** — We know of classical field that is fundamental in physics — the electromagnetic field. Analyses of Bohr and Rosenfeld showed that there are difficulties in having a quantum description of various charged particle phenomena (such as those that occur in atomic physics) while retaining a classical description of the electromagnetic field. One has to quantize the electromagnetic field (e.g., to get Lamb

H. Leutwyler, Il Nuovo Cimento **37**, 556 (1965).

shift correctly); this is independent of any many-particle interpretation that might emerge from quantization.

**IV.** — Because all particles of the same type are the same. What we mean by this is that, for instance, two electrons are identical in every way, regardless of where they came from and what they have been through. The same is true of every other fundamental particle. Let me illustrate this through a rather prosaic story. Suppose we capture a proton from a cosmic ray which we identify as coming from a supernova lying 8 billion light years away. We compare this proton with one freshly created in a particle accelerator here on Earth. And the two are exactly the same! How is this possible? Why are not there errors in proton production? How can two objects, manufactured so far apart in space and time, be identical in all respects? One explanation that might be offered is that there's a sea of proton "stuff" filling the universe and when we make a proton we somehow dip our hand into this stuff and from it mould a proton. Then it's not surprising that protons produced in different parts of the universe are identical: they're made of the same stuff. It turns out that this is roughly what happens. The "stuff" is the proton field or, if one looks closely enough, the quark field.

#### Note on field quantization I

There are two complementary approaches that are typically employed in field quantization.

- a) One can postulate fields as the basic dynamical variables and show that the result can be interpreted in many-body terms.
- **b)** One can start with point-particles as the basic objects of interest and derive (or construct) field operator as an efficient way of organizing the many-particle states.

Here we will work with the first approach as this gets us into the subject quickly. The second approach is often a starting point in non-relativistic field theory that is typically employed in condensed matter physics. Approach **a**) is known as *Quantum Field Theory* (QFT) or *Theory of Quantized Fields*, while **b**) is known as *Second Quantization*.

#### Note on field quantization II

There is a number of different types of quantization schemes, each with its own merits and drawbacks.

Canonical quantization — will also be used as our starting point. It emulates the conventional quantization procedure used in Quantum Mechanics. In particular, time is singled out as a special coordinate and manifest Lorentz invariance is renounced. The advantage of canonical quantization is that it quantizes only physical modes, which ensures that unitarity is manifest. In simple cases such as scalar and fermion fields or quantum electrodynamics (QED) this method is relatively easy to apply. In more complicated (though experimentally important) cases it is impractical.

- ► Gupta-Bleuler or Covariant quantization maintains full Lorentz symmetry (contrary to canonical quantization), which is clearly a great advantage. The disadvantage of this approach is that "ghosts" or unphysical states of negative norm are allowed to propagate in the theory, and are eliminated only when one applies constraints to the state vectors. This approach was historically most successful in QED. It is rather limited in its scope and rarely used beyond QED.
- ► Functional integral will be utilized in the second part of this lecture. It is a simple, intuitive method with a close connection with classical physics (it employs, e.g., Lagrangian density, action functional or Hamilton variational principle). It provides an excellent tool for various semiclassical approximations. In addition, the functional integral is formulated in manifestly Lorentz covariant fashion. Corresponding "ghosts" are killed by another type of "ghosts" (the so called "good ghosts" or Faddeev-Popov ghosts). It is also an ideal bookkeeping tool allowing for a systematic perturbation expansion in terms of the so-called *Feynman diagrams*. The disadvantage of this approach is that functional integration is mathematically delicate operation that may not even exist in Minkowski space.
- ▶ Becchi-Rouet-Stora-Tyutin (BRST) & Batalin-Vilkovisky quantization schemes — are fully covariant quantization methods. They are used in complicated systems, such as non-abelian Yang-Mills theories, string theory or quantum gravity. They can be (and as a rule are) expressed in terms of functional integrals.
- Stochastic quantization is conceptually very different from previous quantization schemes. The main idea is to view Euclidean field theory (i.e., field theory where time variable is analytically continued to imaginary values) as an equilibrium limit of a statistical system coupled to a thermal reservoir. This system evolves in a fictitious time direction *t* (5th parameter) until it reaches equilibrium limit as *t* → ∞. The coupling to a heat reservoir is simulated by means of a stochastic noise. Stochastic quantization is particularly suitable for numerical applications.

## 2.2 Some useful background from quantum mechanics

Let us first recall the familiar path to the quantization of a classical dynamical system in particle mechanics. For the purpose of illustration

we consider a 1-D motion of a particle in a conservative potential. Let q be the (generalized) coordinate of the particle,  $\dot{q} = dq/dt$  the velocity, and  $L(q, \dot{q})$  the Lagrangian. According to Hamilton's principle, the dynamics of the particle is determined by the condition

$$\delta S[q] = \delta \int_{t_1}^{t_2} \mathrm{d}t L(q, \dot{q}) = 0, \qquad (2.2)$$

which provides an actual physical trajectory q(t) from  $(q_1, t_1)$  to  $(q_2, t_2)$ . Eq. (2.2) states that the action functional is stationary around classical trajectory, i.e. small variations from classical path,  $q(t) \rightarrow q(t) + \delta q(t)$ , leave the action unchanged to the first order in the variation.

Hamilton's principle gives us the well known Euler-Lagrange equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0.$$
(2.3)

In order to carry out the formal quantization based on this equation, we rewrite it in the Hamiltonian form, by defining the momentum p conjugate to q as

$$p \equiv \frac{\partial L}{\partial \dot{q}}, \qquad (2.4)$$

and introduce the Hamiltonian via the Legendre transformation

$$H(p,q) = p\dot{q} - L(q,\dot{q}).$$
 (2.5)

Note, that *H* does not dependent on  $\dot{q}$  since

$$dH = (dp)\dot{q} + pd\dot{q} - \frac{\partial L}{\partial q}dq - \frac{\partial L}{\partial \dot{q}}d\dot{q}$$
$$= (dp)\dot{q} - \frac{\partial L}{\partial q}dq. \qquad (2.6)$$

In terms of *H*, the Euler-Lagrange equation can be equivalently rewritten as

$$\{q, H\}_{PB} = \frac{\partial H}{\partial q} = \dot{q},$$
  
$$\{p, H\}_{PB} = -\frac{\partial H}{\partial q} = \dot{p},$$
 (2.7)

where  $\{\cdot, \cdot\}_{PB}$  denotes a Poisson bracket. To quantize (2.7) we let *q* become a Hermitan operator in a Hilbert space and replace *p* by  $-i\partial/\partial q$ , so that the conjugate momentum and coordinate satisfy a commutation relation

$$[q,p] = i\hbar, \qquad (2.8)$$

which corresponds to the classical Poisson bracket  $\{q, p\}_{PB} = 1$ . The dynamics of our particle is contained in the Schrödinger equation

$$H(p,q)\psi(t) = i\frac{\partial\psi(t)}{\partial t}, \qquad (2.9)$$

where  $\psi(t)$  is a wave function (or state vector) in the Hilbert space. In this formulation all time dependence is carried by  $\psi$  while *p* and *q* 

This is analogous to the situation when df(x) = 0, which implies that f(x) is stationary around the extremal point  $x_0$  of f(x), i.e.,  $f(x_0) = f(x_0 + dx)$  to the first order in dx.

are not time dependent. This approach is known as the Schrödinger picture.

Alternatively, we may transfer whole time dependence to the operators q(t) and p(t) while  $\psi$  will be time independent. This is known as *Heisen*berg picture. Both pictures are equivalent as they can be connected via unitarity transformation. In fact, from Schrödinger equation it follows that

$$\psi_S(t) = e^{-iH_S t} \psi_S(0) = e^{-iH t} \psi_H , \qquad (2.10)$$

where the value  $\psi_S(t = 0)$  is set to coincide with  $\psi_H$ . Similarly, operators in both pictures are connected according to prescription

$$O_H(t) = e^{iH_S t} O_S e^{-iH_S t} . (2.11)$$

It is clear that the unitary transformation (2.11) is constructed so that matrix elements of all observables are identical at all times provided they coincide at some reference time  $t_0$  (here  $t_0 = 0$ ). This is precisely what we require in quantum theory, where dynamical problem typically consist in finding, at a later time *t*, matrix elements of operators, which represent physical observables, provided we know the matrix elements at some initial time. In Schrödinger picture this is done by solving Schrödinger equation.

In Heisenberg picture, one solves the equation of motion for the Heisenberg operator  $O_H(t)$ 

$$\frac{dO_H(t)}{dt} = i [H_S, O_H(t)].$$
 (2.12)

which directly follows from (2.11). This can also be alternatively viewed as a consequence of Dirac's quantization condition.

#### Note

▶ As long as we deal with *energy eigenfunctions* and *eigenvalues* in non-relativistic theory, there is a little practical difference between Schrödineger and Heisenberg picture, as in the absence of external time-varying forces we have

$$H_H(t) = H_S \equiv H \,,$$

and hence  $\frac{dH}{dt} = 0$ . As for energy eigenfunctions, the Schrödinger wave function is  $\psi_H(q, t) = e^{-i\omega_n t} u_n(q)$  while the corresponding Heisenberg wave function is simply  $u_n(q)$ . Spectrum is (due to a unitary similarity between both pictures) identical.

▶ In *relativistic field theory*, the Heisenberg picture is more convenient, since the explicit representation of the state vector  $\psi$ is considerably more complicated than in the non-relativistic case (such a  $\psi$  is a solution of the so-called functional Schrödinger equation), and the dynamics of operators is easier to describe and solve (even if only perturabtively) than the dy-

There also exist intermediate pictures, such as Dirac picture or thermo-field dynamics that will be discussed later on.

When  $O_H$  has also explicit time dependence then this generalizes to

$$\frac{\mathrm{d}O_H(t)}{\mathrm{d}t} = i \left[H, O_H(t)\right] + \frac{\partial O_H(t)}{\partial t}.$$

namics of  $\psi$ .

- Lorentz invariance can be more readily implemented in the Heisenberg picture, which puts time together with space coordinates in the field operators. So, one can, for instance, formulate Lorentz covariant field equations. Note also, that time and space are both treated on equal footing, in particular both are *c*-numbers.
- ► In Quantum Mechanics are both pictures unitarily equivalent. This unitary equivalence is guaranteed by the so-called *Stone-von Neumann uniqueness theorem,* which states that all irreducible representations of the canonical commutation relation are for a finite number of degrees of freedom unitarily equivalent to that of Schrödinger.

In QFT is the unitary equivalence violated. This violation can be, in turn related to the concept of *renormalization*.

In the Heisenberg picture it follows that the CCR retain the form

$$[q(t), p(t)] = i, (2.13)$$

which is again dictated by Dirac's quantization condition. For an arbitrary *t* the operators can be represented as

$$\hat{p}(t) = -i \frac{\partial}{\partial q(t)}, \quad \hat{q}(t) = q(t),$$
(2.14)

in *q*-representation, and

$$\hat{p}(t) = p(t), \quad \hat{q}(t) = i \frac{\partial}{\partial p(t)},$$
(2.15)

in *p*-representation.

From (2.12) we can directly write the equations of motion for the canonical variables (the Heisenberg dynamical equations) in the form

$$\frac{\mathrm{d}p(t)}{\mathrm{d}t} = i \left[H, p(t)\right],$$

$$\frac{\mathrm{d}q(t)}{\mathrm{d}t} = i \left[H, q(t)\right]. \qquad (2.16)$$

To completely determine the dynamical problem in Quantum Mechanics, we must still specify the matrix elements of p and q at the initial time.

Let us illustrate the aforemntioned quantization methodology on a simple problem. To this end we consider Lagrangian of the form

$$L = \frac{1}{2}m\dot{q}^2 - \frac{\omega^2}{2}mq^2.$$
 (2.17)

Sub-index *H* and hat over operators will be mostly suppressed further on.

The corresponding action functional is given by

$$S = \int_{t_1}^{t_2} dt \left[ \frac{1}{2} m \dot{q}^2 - \frac{\omega^2}{2} m q^2 \right] = \frac{m}{2} \int_{t_1}^{t_2} dt \left[ \dot{q}^2 - \omega^2 q^2 \right].$$
(2.18)

Requirement that  $\delta S = 0$  yields the equation of motion

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial L}{\partial \dot{q}} - \frac{\partial L}{\partial q} = 0, \qquad (2.19)$$

which reduces to the

$$\ddot{q} + \omega^2 q = 0.$$
 (2.20)

This is the equation of motion in a *configuration space*.

Corresponding equations in the *phase space* are obtained by defining the conjugate momentum p (consider further m = 1)

$$p = \frac{\partial L}{\partial \dot{q}} = m\dot{q} = \dot{q}. \tag{2.21}$$

Ensuing Hamiltonian is defined via Legendre transformation

$$H(p,q) = p\dot{q} - L(q,\dot{q})$$
  
=  $p^2 - \frac{1}{2}p^2 + \frac{\omega^2}{2}q^2 = \frac{1}{2}\left(p^2 + \omega^2 q^2\right).$  (2.22)

This is nothing but the Hamiltonian of linear harmonic oscillator. Hamilton equations of motion read

$$\frac{\mathrm{d}q}{\mathrm{d}t} = \{q, H\}_{PB} = \frac{\partial H}{\partial p} = p,$$

$$\frac{\mathrm{d}p}{\mathrm{d}t} = \{p, H\}_{PB} = -\frac{\partial H}{\partial q} = -\omega^2 q, \qquad (2.23)$$

which are clearly equivalent to the Euler-Lagrange equation (2.20).

We can now pass to Quantum Mechanics by making change

$$\{\cdot,\cdot\}_{PB} \rightarrow -\frac{i}{\hbar} [\cdot,\cdot] , \qquad (2.24)$$

or, in more explicit terms

This can also be written as:  $\{f,g\}_{PB} = d \rightarrow [O_f, O_g] = i\hbar O_d.$ 

$$O_{\{f,g\}_{PB}} = -\frac{i}{\hbar} \left[ O_f, O_g \right] \,. \tag{2.25}$$

Here,  $Q_f$  denotes an operator representation of a classical dynamical function f. This allows to write

$$\begin{aligned} \dot{q} &= \{q, H\}_{PB} = p \rightarrow [\hat{q}, \hat{H}] = i\hbar\hat{p}, \\ \dot{p} &= \{p, H\}_{PB} = -\omega^2 q \rightarrow [\hat{p}, \hat{H}] = i\hbar\omega^2\hat{q}, \end{aligned} (2.26)$$

which is equivalent to the operator (configuration-space) equation (again without using hats)

$$\ddot{q} = -\omega^2 q \,. \tag{2.27}$$

To diagonalize the system of equations (2.26) we define ladder operators

$$a(t) = \frac{\omega q(t) + ip(t)}{\sqrt{2\omega}},$$
  

$$a^{\dagger}(t) = \frac{\omega q(t) - ip(t)}{\sqrt{2\omega}}.$$
(2.28)

These can also be equivalently introduced as

$$\begin{aligned} q(t) &= \frac{1}{\sqrt{2\omega}} \left( a^{\dagger}(t) + a(t) \right) , \\ p(t) &= i \sqrt{\frac{\omega}{2}} \left( a^{\dagger}(t) - a(t) \right) , \end{aligned} \tag{2.29}$$

It is not difficult to see that the the above ladder operators indeed diagonalize the system of equations (2.26), in fact

$$\dot{a}^{\dagger}(t) = -i \left[ a^{\dagger}(t), H \right] = -i \left[ \frac{\omega q(t) - i p(t)}{\sqrt{2\omega}}, H \right]$$
$$= \frac{\omega p(t) + i \omega^2 q(t)}{\sqrt{2\omega}} = i \omega a^{\dagger}(t).$$
(2.30)

By Hermitian conjugation we obtain analogous equation for a(t). Corresponding solutions can be written in the form

$$a^{\dagger}(t) = a^{\dagger}(0)e^{i\omega t},$$
  
$$a(t) = a(0)e^{-i\omega t}.$$
 (2.31)

With these we can rewrite q(t) as

$$q(t) = \frac{1}{\sqrt{2\omega}} \left( a^{\dagger}(0)e^{i\omega t} + a(0)e^{-i\omega t} \right) , \qquad (2.32)$$

and similar formula could be written also for p(t). In terms of a(t) and  $a^{\dagger}(t)$  the Hamiltonian reads

$$H = \frac{1}{2}\omega \left( a^{\dagger}(t)a(t) + a(t)a^{\dagger}(t) \right)$$
  
=  $\frac{1}{2}\omega \left( a^{\dagger}(0)a(0) + a(0)a^{\dagger}(0) \right)$   
=  $\omega \left( a^{\dagger}(0)a(0) + \frac{1}{2} \right).$  (2.33)

There exists yet another advantage by introducing the ladder operators. In particular, from functional analysis is known that if there exist two operators *A* and  $A^{\dagger}$  such that  $[A, A^{\dagger}] = \lambda \in \mathbb{R}^+$  is satisfied, then the eigenvalues of  $A^{\dagger}A$  operator are  $0, \lambda, 2\lambda, 3\lambda, \ldots$ 

Since  $[a(0), a^{\dagger}(0)] = 1$ , we see that the spectrum of *H* is  $\omega_n = \omega(n + 1/2)$  with  $\omega = 0, 1, 2, ...$  By denoting the eigenstates related to  $\omega_n$  as  $|n\rangle$  we

In finite dimensional Hilbert spaces there is no couple of operators A and B such that [A, B] = 1.

can write

$$H|n\rangle = \omega_n |n\rangle = \omega \left(n + \frac{1}{2}\right)|n\rangle, \quad n = 0, 1, \dots$$
 (2.34)

Important property of the spectrum is that it is equidistant, namely  $\omega_n - \omega_{n-1} = \omega$ .

The *lowest* energy state  $|0\rangle$  (also known as *vacuum state* or *ground state*) satisfies

$$H|0\rangle = \omega \left( a^{\dagger}(0)a(0) + \frac{1}{2} \right) |0\rangle = \frac{1}{2}\omega |0\rangle .$$
 (2.35)

Because  $a^{\dagger}(0)a(0) |0\rangle = 0$  we have that

$$\langle 0|a^{\dagger}(0)a(0)|0\rangle = ||a(0)|0\rangle||^2 = 0,$$
 (2.36)

which implies that the vacuum state is annihilated by the a(0) operator.

Suppose now that

$$H\left|n\right\rangle = \omega_{n}\left|n\right\rangle, \qquad (2.37)$$

then by applying  $a^{\dagger}(0)$  to  $|n\rangle$  we get

$$H[a^{\dagger}(0)|n\rangle] = \left( \left[ H, a^{\dagger}(0) \right] + a^{\dagger}(0)H \right) |n\rangle$$
$$= \left( \omega a^{\dagger}(0) + a^{\dagger}(0)\omega_n \right) |n\rangle$$
$$= (\omega + \omega_n)[a^{\dagger}(0)|n\rangle].$$
(2.38)

This implies that  $a^{\dagger}(0) |n\rangle \propto |n+1\rangle$ . Similarly, by applying a(0) to  $|n\rangle$  we obtain

$$H[a(0)|n\rangle] = (\omega_n - \omega)[a(0)|n\rangle].$$
(2.39)

0.

This implies that  $a(0) |n\rangle \propto |n-1\rangle$ , which terminates at  $|0\rangle$  state.

#### Cute note

For energy eigenstates  $|n\rangle$  we can write

$$2 \langle n|H|n \rangle = 2\omega_n = \langle n|p^2|n \rangle + \omega^2 \langle n|q^2|n \rangle$$
$$= ||p|n\rangle ||^2 + ||\omega q|n\rangle ||^2 \ge 2||p|n\rangle ||||\omega q|n\rangle ||.$$

Where last inequality follows from *triangle inequality*.

We now use *virial theorem* which implies that  $\langle n|p|n \rangle = \langle n|q|n \rangle = 0$ . The latter is a direct consequence of the fact that for any operator *A* and any energy eigenstate  $|n\rangle$  we have

$$\langle n | [A, H] | n \rangle = \langle n | AH | n \rangle - \langle n | HA | n \rangle$$
$$= \omega_n \langle n | A| n \rangle - \omega_n \langle n | A| n \rangle =$$

Thus if A = q

$$\langle n | [q, H] | n \rangle = \langle n | i p | n \rangle = 0,$$

or when A = p

$$\langle n | [p, H] | n \rangle = -i\omega \langle n | q | n \rangle = 0.$$

Consequently

$$2\langle n|H|n\rangle \geq 2||p|n\rangle|||\omega q|n\rangle|| \geq 2\omega\Delta p\Delta q \geq \hbar\omega$$
.

So, uncertainty relation prohibits  $\langle n|H|n \rangle = \omega_n$  to be smaller that  $\hbar\omega/2$ . Eigenvalue  $\omega_n = \hbar\omega/2$  represents the so-called zero mode of *H* (in this specific case we call it also *zero-mode fluctuation* or *ground state fluctuation*).

In particular, by applying creation operator on vacuum state we get

$$a^{\dagger}(0) |0\rangle \propto |1\rangle$$
, (2.40)

and generally

$$(a^{\dagger}(0))^n |0\rangle \propto |n\rangle$$
. (2.41)

After normalization of states to the  $\langle n|m \rangle = \delta_{nm}$ , we get

$$|n\rangle = \frac{(a^{\dagger})^n}{\sqrt{n!}} |0\rangle . \qquad (2.42)$$

which can be easily proved by induction.

It is now straightforward to generalize this procedure to *N* degrees of freedom. We introduce *N* Hermitian operators  $q_i(t)$ , i = 1, ..., N in the Heisenberg picture and *N* conjugate momenta  $p_i(t)$ . The dynamics is again given by the 2*N* classical equations of motion

$$\{p_i, H\}_{PB} = -\frac{\partial H}{\partial q_i} = \dot{p}_i,$$
  
$$\{q_i, H\}_{PB} = \frac{\partial H}{\partial p_i} = \dot{q}_i, \quad i = 1, \dots, N.$$
 (2.43)

Again, our goal is to find the matrix elements of  $p_i$  and  $q_i$  at an initial time, say t = 0 with the restriction that

$$[p_i(0), q_j(0)] = -i\delta_{ij},$$

$$[p_i(0), p_j(0)] = 0,$$

$$[q_i(0), q_j(0)] = 0.$$

$$(2.44)$$

By employing Dirac's quantization condition we can from (2.43) write Heisenberg equations of motion in the form

$$\dot{p}_i(t) = i [H, p_i(t)],$$
  
 $\dot{q}_i(t) = i [H, q_i(t)].$  (2.45)

### 2.3 Fields

A *field* is a quantity defined at every point of space x and time t. While classical particle mechanics deals with a finite number of generalized coordinates  $q_i(t)$ , indexed by a discrete label "i", in field theory we are interested in the dynamics of fields  $\phi_a(x, t)$ , where both "a" and "x" are considered as labels. We are thus dealing with a system with an infinite (uncountably infinite) number of degrees of freedom — at least one for each point x in space.

Notice, that the concept of position has been relegated from a dynamical variable in particle mechanics (so called wave mechanics or first quantization) to a mere label in field theory.

#### Example — Electromagnetic field

 $E(\mathbf{x}, t)$  and  $B(\mathbf{x}, t)$ , both of these fields are 3 spatial vectors — 3 *di*mensional vector fields. In covariant treatment of electromagnetism one introduces instead of E and B electromagnetic potential  $A^{\mu}$  $E, B \rightarrow A^{\mu}(\mathbf{x}, t) = (\phi, A) \ (\mu = 0, ..., 3)$ , where  $A^{\mu}$  is a vector in spacetime — 4 *dimensional vector field*. Connection between E, Band  $A^{\mu}$  is done by the Maxwell relation

$$\boldsymbol{E} = -\boldsymbol{\nabla}\phi - \frac{\partial \boldsymbol{A}}{\partial t}, \quad \boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}. \quad (2.46)$$

These defining relations directly imply sourceless Maxwell equations (so called Bianchi identities)

$$\nabla \cdot \boldsymbol{B} = 0, \quad \nabla \times \boldsymbol{E} = -\frac{\partial \boldsymbol{B}}{\partial t}.$$
 (2.47)

To proceed we start again with *Lagrangian*. This is not only convenient starting point for a covariant treatment but it also allows to formulate constructively a field-theoretical systems solely on the basis of required/expected symmetries. Besides, for simple systems the Lagrangian formalism also provides a straightforward passage to Hamiltonian (i.e., canonical) formalism via Legendre transformation.

In the Lagrangian formalism, the dynamics is governed by a Lagrangian, which is a function of  $\phi_i(\mathbf{x}, t)$ ,  $\dot{\phi}(\mathbf{x}, t)$  and  $\nabla \phi_i(\mathbf{x}, t)$ . We change our Lagrangian (*L*) to Lagrangian density ( $\mathcal{L}$ ), i.e.

$$L(\boldsymbol{q}, \dot{\boldsymbol{q}}) \to \int \mathrm{d}^3 \boldsymbol{x} \mathcal{L}(\phi_i(\boldsymbol{x}, t), \partial_\mu \phi_i(\boldsymbol{x}, t)).$$
(2.48)

In principle, we could consider also higher derivative terms (or even non-local interactions), but in all systems, studied in this course, the Lagrangian will be of the form given above. The action is

$$S = \int_{t_1}^{t_2} dt L = \int_{t_1}^{t_2} dt \int d^3 \mathbf{x} \mathcal{L}(\phi_i, \partial_\mu \phi_i)$$
$$= \int d^4 x \mathcal{L}(\phi_i, \partial_\mu \phi_i). \qquad (2.49)$$

In particle mechanics *L* depends on  $q_i$  and  $\dot{q}_i$ , but not  $\ddot{q}_i$ . In field theory we similarly restrict the Lagrangian  $\mathcal{L}$  to  $\phi_i$  and  $\dot{\phi}_i$ . In principle, there is

It should be stressed that (2.47) are not field equations, since there are no sources; rather, they impose constraints on the electric and magnetic fields. nothing to stop  $\mathcal{L}$  from depending on  $\nabla \phi$ ,  $\nabla^2 \phi$ ,  $\nabla^3 \phi$ , ... In cases when we require Lorentz invariance, we will consider only dependence of  $\mathcal{L}$  on  $\nabla \phi$  (this is not needed in non-relativistic context). We will also not consider  $\mathcal{L}$  explicitly dependent on  $x^{\mu}$  (no external fields).

Corresponding equations of motion are obtained via the principle of stationary action (Hamilton's principle)

$$\delta S = \int d^4 x \left[ \frac{\partial \mathcal{L}}{\partial \phi_i} \delta \phi_i + \frac{\partial \mathcal{L}}{\partial (\partial_\mu \phi_i)} \delta (\partial_\mu \phi_i) \right]$$
  
= 
$$\int d^4 x \left[ \frac{\partial \mathcal{L}}{\partial \phi_i} \delta \phi_i - \partial_\mu \left( \frac{\partial \mathcal{L}}{\partial (\partial_\mu \phi_i)} \right) \delta \phi_i + \partial_\mu \left( \frac{\partial \mathcal{L}}{\partial (\partial_\mu \phi_i)} \delta \phi_i \right) \right]. \quad (2.50)$$

We can now neglect the surface term due to condition that  $\delta \phi_i = 0$  on the surface. By the *fundamental lemma of calculus of variations* this leads to the Euler-Lagrange equations of motion for fields  $\phi_i$ 

$$\partial_{\mu} \left( \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi_i)} \right) - \frac{\partial \mathcal{L}}{\partial \phi_i} = 0.$$
 (2.51)

Let us now list a couple of illustrative field systems.

#### ► Example I — Klein-Gordon field

Consider Lagrangian for a real scalar field  $\phi(t, \mathbf{x})$  in the form

$$\mathcal{L} = \frac{1}{2} \eta^{\mu\nu} \partial_{\mu} \phi \partial_{\nu} \phi - \frac{1}{2} m^2 \phi^2$$
$$= \frac{1}{2} \phi^2 - \frac{1}{2} (\nabla \phi)^2 - \frac{1}{2} m^2 \phi^2. \qquad (2.52)$$

For equation of motion we need

$$\frac{\partial \mathcal{L}}{\partial \phi} = -m^2 \phi, \quad \frac{\partial \mathcal{L}}{\partial (\partial_\mu \phi)} = \partial^\mu \phi = (\dot{\phi}, -\nabla \phi). \quad (2.53)$$

By using the Euler-Lagrange equation we arrive at the equation of the motion

$$\ddot{\phi} - \nabla^2 \phi + m^2 \phi = 0 \quad \Leftrightarrow \quad \Box \phi + m^2 \phi = 0. \tag{2.54}$$

This is nothing but the Klein-Gordon equation. In this time, however for a classical field and not for the wave function.

#### ▶ Example II — First order field Lagrangian

As a second example we consider Lagrangian with a complex field that is linear in time derivative (rather than quadratic), namely

$$\mathcal{L} = \frac{i}{2} \left( \psi^* \dot{\psi} - \dot{\psi}^* \psi \right) - \nabla \psi^* \nabla \psi - m \psi^* \psi . \qquad (2.55)$$

For equation of motion we need

$$\frac{\partial \mathcal{L}}{\partial \psi^*} = \frac{i}{2} \dot{\psi} - m\psi, \quad \frac{\partial \mathcal{L}}{\partial \dot{\psi}^*} = -\frac{i}{2} \psi, \quad \frac{\partial \mathcal{L}}{\partial \nabla \psi^*} = -\nabla \psi. \quad (2.56)$$

The corresponding Euler-Lagrange equation thus implies equation of motion

$$i\frac{\partial\psi}{\partial t} = -\nabla^2\psi + m\psi. \qquad (2.57)$$

Note that this equation looks like Schrödinger equation, but it is not. Its interpretation is very different and besides the field  $\psi$  is a classical field with no probabilistic interpretation à la wave function.

#### ► Example III — Maxwell equations

Consider a Lagrangian of the form

$$\mathcal{L} = -\frac{1}{2} (\partial_{\mu} A_{\nu}) (\partial^{\mu} A^{\nu}) + \frac{1}{2} (\partial_{\mu} A^{\mu})^{2} .$$
 (2.58)

The minus sign in front of the gradient term ensures that the kinetic term for  $A_i$  is positive. Note, also that  $\mathcal{L}$  has no kinetic term  $(\dot{A}_0)^2$  for  $A_0$ , so that  $A_0$  can not correspond to a physical degree of freedom. For equation of motion we need to compute

$$\frac{\partial \mathcal{L}}{\partial (\partial_{\mu} A_{\nu})} = -\partial^{\mu} A^{\nu} + \partial^{\nu} (\partial_{\rho} A^{\rho}), \qquad (2.59)$$

which yields the dynamical equation in the form

$$\partial_{\mu} \left( \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} A_{\nu})} \right) = -\partial_{\mu} \left( \partial^{\mu} A^{\nu} - \partial^{\nu} A^{\mu} \right) \equiv \partial_{\mu} F^{\mu\nu} = 0. \quad (2.60)$$

Here we have defined the field strength tensor  $F^{\mu\nu} = (\partial^{\mu}A^{\nu} - \partial^{\nu}A^{\mu})$ .

By identifying now  $A^{\mu}$  with electromagnetic potential and using the relations for electric and magnetic fields

$$\boldsymbol{E} = -\boldsymbol{\nabla} A^0 - \frac{\partial \boldsymbol{A}}{\partial t}, \quad \boldsymbol{B} = \boldsymbol{\nabla} \times \boldsymbol{A}, \quad (2.61)$$

we can check that (2.60) is equivalent to the first set of Maxwell equations, i.e.

$$\nabla \cdot E = 0, \quad \frac{\partial E}{\partial t} = \nabla \times B.$$
 (2.62)

Indeed, for instance

$$\nabla \cdot \boldsymbol{E} = \partial_k E^k = \left\{ E^k = -\partial_k A^0 - \partial_0 A^k = \partial^k A^0 - \partial^0 A^k \right\}$$
$$= \partial_k \partial^k A^0 - \partial_k \partial^0 A^k = \partial_k \left( \partial^k A^0 - \partial^0 A^i \right) = 0. \quad (2.63)$$

The second series of Maxwell equations, i.e.,

$$\nabla \cdot \boldsymbol{B} = 0, \quad \frac{\partial \boldsymbol{B}}{\partial t} = -\nabla \times \boldsymbol{E}, \qquad (2.64)$$

do not correspond to field equations. These merely impose constraints on the electric and magnetic fields. In fact they are equiv-
alent to Bianchi identity

$$\partial_{\gamma}F_{\alpha\beta} + \partial_{\alpha}F_{\beta\gamma} + \partial_{\beta}F_{\gamma\alpha} = 0, \qquad (2.65)$$

which is a simple identity implied by the structure of  $F_{\mu\nu}$ .

It can also be checked that the Lagrangian (2.58) is (upto 4divergence) identical to the Lagrangian

$$\mathcal{L} = -\frac{1}{4} F^{\mu\nu} F_{\mu\nu} \,. \tag{2.66}$$

# 2.4 Quantization of Scalar Field

We will be particularly interested in relativistic field theories. We have seen that for relativistic (scalar) field theories, equations of motion, i.e. Euler-Lagrange equations read

$$\partial_{\mu} \left( \frac{\partial \mathcal{L}}{\partial(\partial_{\mu}\phi_i)} \right) - \frac{\partial \mathcal{L}}{\partial\phi_i} = 0.$$
 (2.67)

Should this equation be covariant under Lorentz transformations,  $\mathcal{L}$  must transform as scalar density (of weight 1), i.e.

$$\mathcal{L}(x) \equiv \mathcal{L}(\phi_i(x), \partial_\mu \phi_i(x)) \xrightarrow{L} \mathcal{L}_L(x) = |\det L| \mathcal{L}(L^{-1}x).$$
(2.68)

Let us construct the simplest free (real-field) scalar theory with maximally second time derivative in equation of motion.

The simplest  $\mathcal{L}$  that is a scalar density and has bounded from below potential energy is

$$\mathcal{L} = \frac{1}{2} \eta^{\mu\nu} \partial_{\mu} \phi(x) \partial_{\nu} \phi(x) - \frac{1}{2} m^2 \phi^2(x). \qquad (2.69)$$

Proof of the fact that  $\boldsymbol{\mathcal{L}}$  is a scalar density is quite simple. First we realize that

$$\phi(x) \xrightarrow{L} \phi_L = \phi(L^{-1}x)$$
  
$$\partial_\mu \phi(x) \xrightarrow{L} (L^{-1})^{\nu}{}_{\mu} \partial_\nu \phi(L^{-1}x). \qquad (2.70)$$

Thus

 $\partial_{\mu}\phi(x)\partial_{\nu}\phi(x)\eta^{\mu\nu}$ 

$$\stackrel{L}{\rightarrow} (L^{-1})^{\alpha}_{\cdot \mu} \partial_{\alpha} \phi(L^{-1}x)(L^{-1})^{\beta}_{\cdot \nu} \partial_{\beta} \phi(L^{-1}x)L^{\mu}_{\ \gamma} \eta^{\gamma \delta} L^{\nu}_{\ \delta}$$

$$= \partial_{\gamma} \phi(L^{-1}x) \partial_{\delta} \phi(L^{-1}x) \eta^{\gamma \delta} .$$

$$(2.71)$$

In addition, the term  $\phi^2(x)$  transforms simply as  $\phi^2(x) \xrightarrow{L} \phi^2(L^{-1}x)$ . Since  $|\det L| = 1$ , the Lagrangian (2.68) is a scalar density. Consequently, the action functional is a Lorentz scalar. In general, a scalar density of weight *w* would transform as

$$\mathcal{L}(x) \xrightarrow{L} \mathcal{L}_{\boldsymbol{L}}(x) = |\det \boldsymbol{L}|^{w} \mathcal{L}(\boldsymbol{L}^{-1}x).$$

As before, the link between the Lagrangian formalism and canonical quantum theory is established via Hamiltonian formalism. To this end, we start by defining *the conjugate momentum*  $\pi(x)$  to field  $\phi(x)$  as

$$\pi(x) = \frac{\partial \mathcal{L}}{\partial \dot{\phi}(x)} = \frac{\delta S[\phi]}{\delta \dot{\phi}(x)}.$$
 (2.72)

This should not be confused with total (conserved) momentum, which will be defined shortly.

The Hamiltonian density is then given by

$$\mathcal{H}(\pi(x),\phi(x)) \equiv \mathcal{H}(x) = \pi(x)\dot{\phi}(x) - \mathcal{L}(x), \qquad (2.73)$$

where, as in classical mechanics, we eliminate  $\dot{\phi}(x)$  in favour of  $\pi(x)$  everywhere in  $\mathcal{H}(x)$ . The *Hamiltonian* is then the simply

$$H = \int \mathrm{d}^3 \boldsymbol{x} \,\mathcal{H}(x) \,. \tag{2.74}$$

Quantization starts by identifying commutators via Poisson brackets. In particular, we know that

$$-\frac{i}{\hbar} \left[ O_f, O_g \right] = O_{\{f,g\}_{PB}}.$$
(2.75)

#### Poisson brackets in field theory

For two functions f and g that depend on phase-space and time variables their Poisson bracket  $\{f, g\}_{PB}$  is another function that depends on phase space and time.

Given two functions  $f(p_i, q_i, t)$  and  $g(p_i, q_i, t)$  with generalized momenta  $p_1, \ldots, p_N$ , generalized positions  $q_2, \ldots, q_N$  and time t, the Poisson bracket takes the form

$$\{f,g\}_{PB} = \sum_{i=1}^{N} \left[ \frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial f}{\partial p_i} \frac{\partial g}{\partial q_i} \right].$$

Here it is implicit that time arguments are both in functions f, g and phase-space variables identical. As a particular case one has

$$\{q_k, p_l\}_{PB} = \delta_{kl}$$

Passage to continuous degrees of freedom — i.e. *fields*, is obtained by formally replacing

$$q_{i}(t) \rightarrow \phi_{a}(\mathbf{x},t), \quad p_{i}(t) \rightarrow \pi_{a}(\mathbf{x},t),$$

$$\frac{\partial}{\partial q_{i}(t)} \rightarrow \frac{\delta}{\delta \phi_{a}(\mathbf{x},t)}, \quad \frac{\partial}{\partial p_{i}(t)} \rightarrow \frac{\delta}{\delta \pi_{a}(\mathbf{x},t)},$$

$$\sum_{i=1}^{N} \rightarrow \sum_{a} \int d^{3}\mathbf{x}.$$

With this the Poisson brackets between two functionals *A* and *B* 

defined on the field phase space read

$$\{A(\pi,\phi),B(\pi,\phi)\}_{PB} = \sum_a \int \mathrm{d}^3 \boldsymbol{x} \left[ \frac{\delta A}{\delta \phi_a(\boldsymbol{x})} \frac{\delta B}{\delta \pi_a(\boldsymbol{x})} - \frac{\delta A}{\delta \pi_a(\boldsymbol{x})} \frac{\delta B}{\delta \phi_a(\boldsymbol{x})} \right],$$

(time variable is the same on both sides and is customarily omitted). In particular, for canonical field variables we obtain

$$\{\phi_a(\mathbf{x}), \pi_b(\mathbf{y})\}_{PB} = \delta_{ab}\delta(\mathbf{y} - \mathbf{x}).$$

So, that in the Shrödinger picture the canonical commutation relation becomes  $[\phi(\mathbf{x}), \pi(\mathbf{x}')] = i\delta(\mathbf{x} - \mathbf{x}')$ .

In the second step, we construct Hamiltonian

$$H = \int d^3 \boldsymbol{x} \left[ \pi(x) \dot{\phi}(x) - \mathcal{L}(x) \right]$$
  
= 
$$\int d^3 \boldsymbol{x} \pi(x) \dot{\phi}(x) - L. \qquad (2.76)$$

Since in our case  $\pi(x) = \dot{\phi}(x)$ , we get

$$H = \frac{1}{2} \int d^3 \mathbf{x} \left[ \pi(\mathbf{x})^2 + (\nabla \phi(\mathbf{x}))^2 + m^2 \phi(\mathbf{x})^2 \right].$$
 (2.77)

At this stage we can pass to the Heisenberg picture

$$\phi(\mathbf{x}) \rightarrow \phi(\mathbf{x}, t) \equiv \phi(x) = e^{iHt} \phi(\mathbf{x}) e^{-iHt} . \qquad (2.78)$$

(we assume that Heisenberg and Schrödinger picture coincide at the reference time  $t_0 = 0$ ). Similarly for  $\pi(\mathbf{x})$ 

$$\pi(\mathbf{x}) \to \pi(x) = e^{iHt} \pi(\mathbf{x}) e^{-iHt}$$
 (2.79)

Generally, we can derive equal-time commutation relations

$$[\phi(\mathbf{x},t),\pi(\mathbf{x}',t)] = i\delta(\mathbf{x}-\mathbf{x}'),$$
  
$$[\phi(\mathbf{x},t),\phi(\mathbf{x}',t)] = [\pi(\mathbf{x},t),\pi(\mathbf{x}',t)] = 0.$$
(2.80)

Equations of motion for Heisenberg picture fields are then dictated by the Heisenberg-Hamilton relations. The first of these relations is

$$\dot{\phi}(x) = i [H, \phi(x)] = i \int d^3 x' [\mathcal{H}(x', t), \phi(x, t)].$$
 (2.81)

Starting with Schrödinger picture is merely historical coincidence. One could use Dirac's quantization prescription to set up Heisenberg picture directly without going via Schrödinger picture. To this end we need to evaluate  $[\mathcal{H}(\mathbf{x}', t), \phi(\mathbf{x}, t)]$ . One has

$$[\mathcal{H}(\mathbf{x}',t),\phi(\mathbf{x},t)] = \frac{1}{2} \left[ \pi^2(\mathbf{x}',t) + (\nabla'\phi(\mathbf{x}',t))^2 + m^2\phi^2(\mathbf{x}',t),\phi(\mathbf{x},t) \right] \\ = \frac{1}{2} \left[ \pi^2(\mathbf{x}',t),\phi(\mathbf{x},t) \right] \\ = \frac{1}{2} \pi(\mathbf{x}',t) \left[ \pi(\mathbf{x}',t),\phi(\mathbf{x},t) \right] \\ + \frac{1}{2} \left[ \pi(\mathbf{x}',t),\phi(\mathbf{x},t) \right] \pi(\mathbf{x}',t) \\ = -i\pi(\mathbf{x}',t)\delta(\mathbf{x}-\mathbf{x}').$$
(2.82)

Thus

$$[H,\phi(x,t)] = -i \int d^3x' \pi(x',t) \delta(x-x') = -i\pi(x,t), \qquad (2.83)$$

which leads to

$$\dot{\phi}(\mathbf{x},t) = -i(i\pi(\mathbf{x},t)) = \pi(\mathbf{x},t).$$
 (2.84)

Similarly, the second relation reads

$$\dot{\pi}(\mathbf{x},t) = i [H,\pi(\mathbf{x},t)] = i \int d^3 \mathbf{x}' [\mathcal{H}(\mathbf{x}',t),\pi(\mathbf{x},t)] .$$
(2.85)

To evaluate this we need

$$[\mathcal{H}(\mathbf{x}',t),\pi(\mathbf{x},t)] = \frac{1}{2} \left[ (\nabla'\phi(\mathbf{x}',t))^2,\pi(\mathbf{x},t) \right] \\ + \frac{1}{2}m^2 \left[ \phi^2(\mathbf{x}',t),\pi(\mathbf{x},t) \right] \\ = i\nabla'\phi(\mathbf{x}',t)\nabla'\delta(\mathbf{x}-\mathbf{x}') \\ + im^2\phi(\mathbf{x}',t)\delta(\mathbf{x}-\mathbf{x}'), \qquad (2.86)$$

and hence

$$[H, \pi(\mathbf{x}, t)] = i \int d^3 \mathbf{x}' \left[ \nabla' \phi(\mathbf{x}', t) \nabla' \delta(\mathbf{x} - \mathbf{x}') + m^2 \phi(\mathbf{x}', t) \delta(\mathbf{x} - \mathbf{x}') \right]$$
$$= i \left[ -\nabla^2 \phi(\mathbf{x}, t) + m^2 \phi(\mathbf{x}, t) \right].$$
(2.87)

This leads to the second equation of motion of the form

$$\dot{\pi}(\boldsymbol{x},t) = \boldsymbol{\nabla}^2 \phi(\boldsymbol{x},t) - m^2 \phi(\boldsymbol{x},t).$$
(2.88)

Recall that  $\dot{\phi}(\mathbf{x}, t) = \pi(\mathbf{x}, t)$ , then

$$\ddot{\phi}(\mathbf{x},t) = \dot{\pi}(\mathbf{x},t) = \nabla^2 \phi(\mathbf{x},t) - m^2 \phi(\mathbf{x},t).$$
 (2.89)

This is an equation of motion for the Heisenberg field, which can be cast into more familiar form

$$\ddot{\phi} - \nabla^2 \phi = -m^2 \phi \quad \Leftrightarrow \quad \partial_\mu \partial^\mu \phi + m^2 \phi = 0.$$
 (2.90)

Which can be succinctly rewritten as

$$\left(\Box + m^2\right)\phi = 0. \tag{2.91}$$

#### Momentum operator and energy momentum tensor

Our Hamiltonian reads

$$H = \int d^3 \boldsymbol{x} \left[ \pi(\boldsymbol{x}) \dot{\phi}(\boldsymbol{x}) - \mathcal{L}(\boldsymbol{x}) \right]$$
  
= 
$$\int d^3 \boldsymbol{x} \, \dot{\phi}^2(\boldsymbol{x}, t) - L(\boldsymbol{x}, t) \,. \qquad (2.92)$$

With this the Heisenberg field obeys the evolution equation  $\phi(\mathbf{x}, t) = e^{iHt}\phi(\mathbf{x}, 0)e^{-iHt}$ , which can be equivalently rewritten as

$$\phi(x, t - \tau) = e^{-iH\tau} \phi(x, t) e^{iH\tau} .$$
(2.93)

We can now ask question: "How does operator P, that affects spatial transformation, look like?" If we translate the physical system by a spatial displacement a, then  $\phi(x, t) \rightarrow \phi(x - a, t)$ . Idea is that the momentum operator P should be the generator of these translations. In other words, we require that

$$e^{i\boldsymbol{P}\cdot\boldsymbol{a}}\phi(\boldsymbol{x},t)e^{-i\boldsymbol{P}\cdot\boldsymbol{a}} = \phi(\boldsymbol{x}-\boldsymbol{a},t).$$
(2.94)

Let a be infinitesimal, then we can write (2.94) as

$$\phi(\boldsymbol{x},t) + i\left[\boldsymbol{P}\cdot\boldsymbol{a},\phi(\boldsymbol{x},t)\right] + O(\boldsymbol{a}^2). \tag{2.95}$$

On the other hand, according to Taylor's expansion

$$\phi(\mathbf{x} - \mathbf{a}, t) = \phi(\mathbf{x}, t) - \mathbf{a} \cdot \nabla \phi(\mathbf{x}, t) + O(\mathbf{a}^2).$$
(2.96)

This implies that

$$i[\mathbf{P} \cdot \mathbf{a}, \phi(\mathbf{x}, t)] = -\mathbf{a} \cdot \nabla \phi(\mathbf{x}, t).$$
(2.97)

Since *a* is arbitrary, we have

$$i\left[\boldsymbol{P}^{k},\phi(\boldsymbol{x},t)\right] = -\boldsymbol{\nabla}_{k}\phi(\boldsymbol{x},t). \qquad (2.98)$$

To construct  $P^k$ , we observe that

$$\begin{bmatrix} \pi(\mathbf{x}', t) \nabla'_k \phi(\mathbf{x}', t), \phi(\mathbf{x}, t) \end{bmatrix} = [\pi(\mathbf{x}', t), \phi(\mathbf{x}, t)] \nabla'_k \phi(\mathbf{x}', t)$$
$$= -i\delta(\mathbf{x} - \mathbf{x}') \nabla'_k \phi(\mathbf{x}', t),$$
(2.99)

and so we can choose

$$\boldsymbol{P}^{k} = -\int \mathrm{d}^{3}\boldsymbol{x}' \boldsymbol{\pi}(\boldsymbol{x}',t) \boldsymbol{\nabla}_{k} \boldsymbol{\phi}(\boldsymbol{x}',t) \,. \tag{2.100}$$

The sign in the generator is dictated by the presumed covariant form

$$e^{-iP_{\mu}a^{\mu}}\phi(\mathbf{x},t)e^{iP_{\mu}a^{\mu}} = \phi(x-a).$$

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Indeed, in this case

$$\begin{bmatrix} \boldsymbol{P}^{k}, \phi(\boldsymbol{x}, t) \end{bmatrix} = -\int d^{3}\boldsymbol{x}'[\pi(\boldsymbol{x}, t)\boldsymbol{\nabla}_{k}\phi(\boldsymbol{x}', t), \phi(\boldsymbol{x}, t)]$$
$$= (-1)(-i)\int d^{3}\boldsymbol{x}'\delta(\boldsymbol{x} - \boldsymbol{x}')\boldsymbol{\nabla}_{k}\phi(\boldsymbol{x}', t) = i\boldsymbol{\nabla}_{k}\phi(\boldsymbol{x}, t). \quad (2.101)$$

This is precisely what we have required for  $P^k$ . Relation (2.100) thus fixes  $P^k$  modulo additive *c*-number (this point will be discussed shortly).

By using the fact that  $\nabla_k = \partial_k = -\partial^k$ , (k = 1, 2, 3) we can write

$$\boldsymbol{P}^{k} = \int \mathrm{d}^{3}\boldsymbol{x} \,\pi(\boldsymbol{x},t) \partial^{k} \phi(\boldsymbol{x},t) \,. \tag{2.102}$$

In addition, we can check that  $P^k$  is independent of *t* and so it represents a conserved quantity. To see this let us consider the commutator [H, P]. Recalling that

$$H = \int d^3 \mathbf{x} \left[ \frac{1}{2} \pi^2(\mathbf{x}, t) + \frac{1}{2} (\nabla \phi(\mathbf{x}, t))^2 + \frac{1}{2} m^2 \phi^2(\mathbf{x}, t) \right].$$
(2.103)

we can directly write

$$[H, P] = -\int d^{3}x d^{3}x' \left[ \pi(x, t)\partial^{k}\phi(x, t), \left(\frac{1}{2}\pi^{2}(x', t) + \frac{1}{2}(\nabla\phi(x', t))^{2} + \frac{1}{2}m^{2}\phi^{2}(x', t)\right) \right]$$

$$= \int d^{3}x' \left[ H, \pi(x', t) \right] \partial^{'k}\phi(x', t) + \pi(x', t) \left[ H, \partial^{'k}\phi(x, t) \right]$$

$$= \int d^{3}x - i\pi(x, t)\partial^{k}\phi(x, t) + \pi(x, t)\partial^{k} \underbrace{[H, \phi(x, t)]}_{-i\pi(x, t)}$$

$$= -i\int d^{3}x' \left[ \left( \nabla'\nabla'\phi(x', t) - m^{2}\phi(x', t) \right) \partial^{k}\phi(x', t) + \pi(x', t)\partial^{'k}\pi(x', t) \right]$$

$$= -i\int d^{3}x \nabla\nabla\phi(x, t)\nabla_{k}\phi(x, t)$$

$$= -i\int d^{3}x \underbrace{\left\{ -\frac{1}{2}\nabla_{k} \left[ \nabla_{l}\phi(x, t)\nabla_{l}\phi(x, t) \right] \right\}}_{\text{surface term}}$$

$$= 0. \qquad (2.104)$$

Thus, for a field that at each fixed *t* and  $|\mathbf{x}| \rightarrow \infty$  goes quickly to zero, the commutator of  $[H, \mathbf{P}] = 0$ .

Let us now set  $P^0 = H$ , then we can combine the above results for H and P to a single 4-vector

$$P^{\mu} = (P^{0}, \mathbf{P}) = \int d^{3}x T^{0\mu}(x), \qquad (2.105)$$

where the tensor

$$T^{\mu\nu} = \partial^{\mu}\phi\partial^{\nu}\phi - g^{\mu\nu}\mathcal{L}(\phi(x),\dot{\phi}(x)).$$
(2.106)

It is easy to see that such  $T^{\mu\nu}$  provides a correct 4-momentum. In fact, from (2.106) we have that

$$T^{00} = \partial^0 \phi \partial^0 \phi - \mathcal{L} = \partial_t \phi \partial_t \phi - \mathcal{L} = \pi \dot{\phi} - \mathcal{L} = \mathcal{H}, \qquad (2.107)$$

and

$$T^{0k} = \partial^0 \phi \partial^k \phi = -\dot{\phi} \nabla_k \phi = -\pi \nabla_k \phi. \qquad (2.108)$$

This consistently implies both  $H = P^0$  and  $P^k$ . In addition, from the equation of motion it follows that

$$\partial_{\mu}T^{\mu\nu} = 0. \qquad (2.109)$$

Indeed, by using the explicit form for  $\mathcal{L}$  given by (2.69) we have

$$\partial_{\mu}T^{\mu\nu} = \partial_{\mu} \left[ \partial^{\mu}\phi\partial^{\nu}\phi - g^{\mu\nu} \left( \frac{1}{2} (\partial_{\alpha}\phi)^{2} - \frac{1}{2}m^{2}\phi^{2} \right) \right]$$
$$= \underbrace{(\partial_{\mu}\partial^{\mu}\phi)}_{-m^{2}\phi} \partial^{\nu}\phi + \partial^{\mu}\phi\partial_{\mu}\partial^{\nu}\phi - (\partial^{\nu}\partial_{\alpha}\phi)\partial^{\alpha}\phi + m^{2}\phi\partial^{\nu}\phi$$
$$= -m^{2}\phi\partial^{\nu}\phi + m^{2}\phi\partial^{\nu}\phi = 0, \qquad (2.110)$$

Let us finally observe that (2.105) can be rewritten in explicitly covariant manner, so that ensuing  $P^{\mu}$  will be a genuine 4-vector. In particular, we can write (2.105) as

$$P^{\mu} = (P^{0}, \mathbf{P}) = \int dV n_{\mu} T^{\mu\nu}(x). \qquad (2.111)$$

Here, the measure dV is over the space-like slice (of the 4*D* spacetime) that is orthogonal to the unit time-like vector  $n^{\mu}$ . We claim that  $P^{\mu}$  transforms covariantly under a change of  $n^{\mu}$ , i.e.,  $P^{\mu}$  is a genuine Lorentzian 4-vector. To see this, we write

$$\int d^3 \mathbf{x} T^{0\mu}(x) = \int d^4 x \,\delta(x_0) T^{0\mu}(x) = \int d^4 x \left[ \frac{\partial}{\partial x^0} \theta(x_0) \right] T^{0\mu}(x)$$
$$= \int d^4 x \frac{\partial}{\partial x^\nu} \theta(n_0^\alpha x_\alpha) T^{\nu\mu}(x).$$
(2.112)

Here,  $n_0^{\alpha} = (1, 0, 0, 0)$  is a time-like unit vector that is manifestly orthogonal to the space-like slice over which we integrate. Now, we relabel  $x^{\mu}$  in (2.112) to  $x'^{\mu}$  and take the Lorentz transformation  $x^{\mu} \stackrel{L}{\rightarrow} x'^{\mu} = L^{\mu}_{\cdot\nu} x^{\nu}$ .

With this we can write

$$\int d^{4}x' \frac{\partial}{\partial x'^{\nu}} \theta(n_{0}^{\alpha}x'_{\alpha})T^{\nu\mu}(x')$$

$$= \int d^{4}x |\det L| L_{\nu}^{\cdot\sigma} \frac{\partial}{\partial x^{\sigma}} \theta(n_{0,\alpha}L_{\cdot\beta}^{\alpha}x^{\beta}) L_{\cdot\gamma}^{\nu}L_{\cdot\delta}^{\mu}T^{\gamma\delta}(\underbrace{L^{-1}x'}_{x})$$

$$= \int d^{4}x \eta_{\gamma}^{\sigma} \frac{\partial(n_{0,\alpha}L_{\cdot\beta}^{\alpha}x^{\beta})}{\partial x^{\sigma}} \delta(n_{0,\alpha}L_{\cdot\beta}^{\alpha}x^{\beta}) L_{\cdot\delta}^{\mu}T^{\gamma\delta}(x)$$

$$= L_{\cdot\delta}^{\mu} \int d^{4}x n_{\sigma}' \delta(n'x) T^{\sigma\delta}(x)$$

$$= L_{\cdot\delta}^{\mu} \int dV n_{\sigma}' T^{\sigma\delta}(x), \qquad (2.113)$$

with  $n'_{\nu} = L^{\mu}_{\cdot\nu} n_{0,\mu}$  (which equivalently means that  $n'^{\nu} = (L^{-1})^{\nu}_{\cdot\mu} n^{\mu}_{0}$ ). So, that finally

$$P^{\mu}(n_{0}) = P^{\mu}(Ln') = L^{\mu}_{\cdot \alpha} \int dV n'_{\beta} T^{\beta \alpha}(x) = L^{\mu}_{\cdot \alpha} P^{\alpha}(n'). \quad (2.114)$$

Thus, the 4-vector  $P^{\mu}$  defined by (2.111) transforms as a true relativistic 4-vector under a change of the space-like slice over which we integrate. The order 2 (and type (2,0)) tensor  $T^{\mu\nu}(x)$  is called *energy-momentum tensor* and in this particular case it satisfies the symmetry condition  $T^{\mu\nu} = T^{\nu\mu}$ .

### **Particle interpretation**

Let us now Fourier decompose  $\phi(x)$  as

$$\phi(x) = \int d^4 p e^{-ipx} \tilde{\phi}(p) \,. \tag{2.115}$$

With this we get

$$(\Box + m^2)\phi(x) = 0 \quad \Rightarrow \quad \int d^4 p e^{-ipx} (p^2 - m^2)\tilde{\phi}(p) = 0$$
$$\Rightarrow \quad (p^2 - m^2)\tilde{\phi}(p) = 0. \tag{2.116}$$

Solution of this equation has the generic form

$$\tilde{\phi}(p) = f(p)\delta(p^2 - m^2)$$

$$= f(p)\frac{\delta(p_0 + \sqrt{p^2 + m^2})}{2\sqrt{p^2 + m^2}} + f(p)\frac{\delta(p_0 - \sqrt{p^2 + m^2})}{2\sqrt{p^2 + m^2}}.$$
 (2.117)

Here  $n_{\beta}$  denotes time-like 4-vector orthogonal to space-like slice over which we integrate. Note that space-like property of vectors is preserved under proper Lorentz transformations. Here f(p) is an arbitrary function that is not zero at  $p^2 = m^2$ . Eq. (2.116) implies that that  $\phi(x)$  can be written in the form

$$\phi(x) = \int \frac{d^4p}{2\omega_p} e^{-ipx} [f(p)\delta(p_0 + \omega_p) + f(p)\delta(p_0 - \omega_p)]$$
  
$$= \int \frac{d^3p}{2\omega_p} \left[ e^{-i\omega_p t_0 + ipx} f(\omega_p, p) + e^{i\omega_p t_0 + ipx} f(-\omega_p, p) \right]$$
  
$$= \int \frac{d^3p}{2\omega_p} \left[ e^{-ipx} f(p) + e^{ipx} g(p) \right]. \qquad (2.118)$$

Here we have set  $g(p) = f(-\omega_p, -p)$ . So we can finally rewrite it as

$$\phi(x) = \int \frac{d^3p}{(2\pi)^3 2\omega_p} \left( a(p)e^{-ipx} + b(p)e^{ipx} \right) , \qquad (2.119)$$

where

$$a(p) = (2\pi)^3 f(p), \quad b(p) = (2\pi)^3 g(p).$$
 (2.120)

By requiring that  $\phi$  is Hermitian (in order to have Hermitian Hamiltonian), we have that  $b(p) = a^{\dagger}(p)$ , which gives

$$\phi(x) = \int \frac{\mathrm{d}^3 p}{(2\pi)^3 2\omega_p} \left[ a(p) e^{-ipx} + a^{\dagger}(p) e^{ipx} \right].$$
(2.121)

Similarly for conjugate field momentum  $\pi(x) = \dot{\phi}(x)$ , we obtain

$$\pi(x) = \dot{\phi}(x) = \int \frac{\mathrm{d}^{3} p}{(2\pi)^{3} 2\omega_{p}} \left[ (-i\omega_{p})a(p)e^{-ipx} + i\omega_{p}a^{\dagger}(p)e^{ipx} \right] \\ = -\frac{i}{2} \int \frac{\mathrm{d}^{3} p}{(2\pi)^{3}} \left[ a(p)e^{-ipx} - a^{\dagger}(p)e^{ipx} \right].$$
(2.122)

The measure in the integral (2.121) is manifestly Lorentz invariant. Indeed

$$\frac{\mathrm{d}^{3}\boldsymbol{p}}{(2\pi)^{3}2\omega_{\boldsymbol{p}}} = \frac{\mathrm{d}^{4}p}{(2\pi)^{4}}2\pi\delta(p^{2}-m^{2})\theta(p^{0})\,.$$

At this stage we recall that the canonical commutation relations read

$$[\phi(\mathbf{x},t),\pi(\mathbf{y},t)] = [\phi(\mathbf{x},t),\dot{\phi}(\mathbf{y},t)] = i\delta(\mathbf{x}-\mathbf{y})$$
  
$$[\phi(\mathbf{x},t),\phi(\mathbf{y},t)] = [\pi(\mathbf{x},t),\pi(\mathbf{y},t)] = 0.$$
 (2.123)

From these one can compute commutation relations for a(p) and  $a^{\dagger}(p)$ . It is not difficult to see that the following holds

$$\begin{bmatrix} a(p), a^{\dagger}(p') \end{bmatrix} = (2\pi)^3 2\omega_p \delta(\mathbf{p} - \mathbf{p}')$$

$$\begin{bmatrix} a(p), a(p') \end{bmatrix} = \begin{bmatrix} a^{\dagger}(p), a^{\dagger}(p') \end{bmatrix} = 0.$$
(2.124)

The consistency check can be done as follows. First, we define the notation

$$\sum_{\boldsymbol{p}} = \int \frac{\mathrm{d}^{3}\boldsymbol{p}}{(2\pi)^{3}2\omega_{p}},$$
  
$$\delta_{\boldsymbol{p}\boldsymbol{p}'} = (2\pi)^{3}2\omega_{p}\delta(\boldsymbol{p}-\boldsymbol{p}'). \qquad (2.125)$$

With these, we have, for instance

$$\sum_{\boldsymbol{p}'} \delta_{\boldsymbol{p}\boldsymbol{p}'} f(\boldsymbol{p}') = f(\boldsymbol{p}),$$

$$\left[a(\boldsymbol{p}), a^{\dagger}(\boldsymbol{p}')\right] = \delta_{\boldsymbol{p}\boldsymbol{p}'}.$$
(2.126)

In addition, the field operators acquire succinct forms

$$\phi(x) = \sum_{p} \left( a(p)e^{-ipx} + a^{\dagger}(p)e^{ipx} \right)$$
(2.127)

and

$$\pi(x) = \dot{\phi}(x) = \sum_{p} (-i\omega_p) \left( a(p)e^{-ipx} - a^{\dagger}(p)e^{ipx} \right).$$
(2.128)

Now we set  $x \equiv (t, \mathbf{x})$  and  $y \equiv (t, \mathbf{y})$ . With this convention we can write

$$\begin{aligned} \left[\phi(x), \pi(y)\right] &= \sum_{pp'} (-i\omega_{p'}) \left[a(p)e^{-ipx}, (-a^{\dagger}(p))e^{ip'y}\right] \\ &+ (-i\omega_{p'}) \left[a^{\dagger}(p)e^{ipx}, a(p)e^{-ip'y}\right] \\ &= \sum_{p} \left[(i\omega_{p})e^{ip(x-y)} + (i\omega_{p})e^{-ip(x-y)}\right] \\ &= \int \frac{\mathrm{d}^{3}p}{(2\pi)^{3}} \frac{i2\omega_{p}}{2\omega_{p}} e^{ip(x-y)} \\ &= i\delta(x-y) \,. \end{aligned}$$
(2.129)

Similarly, it can be checked that

$$[\phi(x), \phi(y)] = [\pi(x), \pi(y)] = 0.$$
(2.130)

# Energy — Hamiltonian

Hamiltonian can be written in the form

$$H = \int d^3 x \underbrace{\frac{1}{2} \pi^2(x)}_{H_1} + \underbrace{\frac{1}{2} (\nabla \phi(x))^2}_{H_2} + \underbrace{\frac{m^2 \phi^2}_{H_3}}_{H_3}.$$
 (2.131)

Let us now compute the respective terms explicitly in terms of mode operators *a* and  $a^{\dagger}$ :

$$H_{1} = \int d^{3}x \frac{1}{2}\pi^{2}$$

$$= \frac{1}{2} \sum_{pp'} (-i\omega_{p})(-i\omega_{p'}) \int d^{3}x \left[ a(p)a(p')e^{-i(p+p')x} - a(p)a^{\dagger}(p')e^{-i(p-p')x} + a^{\dagger}(p)a^{\dagger}(p')e^{i(p+p')x} - a^{\dagger}(p)a(p')e^{i(p-p')x} \right]$$

$$= \frac{1}{2} \sum_{pp'} (-\omega_{p}\omega_{p'}) \left[ -a(p)a^{\dagger}(p')(2\pi)^{3}\delta^{3}(p-p') - a^{\dagger}(p)a(p')(2\pi)^{3}\delta^{3}(p-p') \right]$$

$$= \frac{1}{4} \sum_{p} \omega_{p} \left[ a(p)a^{\dagger}(p) + a^{\dagger}(p)a(p) \right]. \qquad (2.132)$$

We stress that this result represents only *time independent* contribution to  $H_1$ . Similarly we can compute time independent contributions to  $H_2$  and  $H_3$ , namely

$$H_{2} = \frac{1}{2} \int d^{3}x (\nabla \phi)^{2}$$
  

$$= \frac{1}{2} \sum_{pp'} (ip)(-ip') \int d^{3}x [a(p)a^{\dagger}(p')e^{-i(p-p')x} + a^{\dagger}(p)a(p')e^{i(p-p')x}]$$
  

$$= \frac{1}{2} \sum_{pp'} pp'(2\pi)^{3}\delta^{3}(p-p')[a(p)a^{\dagger}(p') + a^{\dagger}(p)a(p')]$$
  

$$= \frac{1}{2} \sum_{p} \frac{p^{2}}{2\omega_{p}} \left[ a(p)a^{\dagger}(p) + a^{\dagger}(p)a(p) \right], \qquad (2.133)$$

$$H_3 = \frac{1}{2} \sum_p \frac{m^2}{2\omega_p} \left[ a(p) a^{\dagger}(p) + a^{\dagger}(p) a(p) \right] .$$
 (2.134)

which finally gives

$$H = H_1 + H_2 + H_3 = \frac{1}{2} \sum_{p} \omega_p \left( a(p) a^{\dagger}(p) + a^{\dagger}(p) a(p) \right). \quad (2.135)$$

We could rewrite this as

$$\sum_{\boldsymbol{p}} \omega_{\boldsymbol{p}} \left( a^{\dagger}(p) a(p) + \frac{1}{2} \delta_{\boldsymbol{p} \boldsymbol{p}} \right),$$

which mimics the linear harmonic oscillator, though now we have sum of infinitely many of them and the contribution from  $\frac{1}{2}\omega_{p}\delta_{pp}$  diverges.

## Spatial momentum

Spatial momentum can be written as

$$\boldsymbol{P} = -\int \mathrm{d}^3 \boldsymbol{x} \, \pi(\boldsymbol{x}) \boldsymbol{\nabla} \phi(\boldsymbol{x}) \,. \tag{2.136}$$

It is normally tedious to do this computation in its full length. But we can take advantage that H is time independent and drop all time-dependent terms because these must cancel anyway. Analogous calculation as for H gives

$$P = \frac{1}{2} \sum_{p} p \left[ a(p) a^{\dagger}(p) + a^{\dagger}(p) a(p) \right] , \qquad (2.137)$$

which does not suffer with vacuum divergences. Together with *H*, we can form four-vector

$$P^{\mu} = \frac{1}{2} \sum_{p} p^{\mu} \left[ a(p) a^{\dagger}(p) + a^{\dagger}(p) a(p) \right].$$
 (2.138)

## Particle interpretation

Similarly as in linear harmonic oscillator, the physical states of our quantum system are excitations over a ground state, which we identify with the vacuum state  $|0\rangle$ . Here  $|0\rangle$  satisfies  $a(p)|0\rangle = 0$  for all p.

#### Ground state and excited states

The fact that the *ground state* must be annihilated by a(p) can be easily understood via similar reasoning as done for linear harmonic oscillator.

We first denote the ground state as  $|0\rangle$ , then

$$H|0\rangle = \omega_0|0\rangle,$$

where  $\omega_0$  is the *minimal eigenvalue* of *H*, which by positive definiteness of *H* cannot be negative.

We further note that

$$[H, a(p)] = \sum_{p'} [a^{\dagger}(p')a(p'), a(p)] = -\omega_p a(p),$$

which implies that

$$Ha(p)|0\rangle = \left[a(p)H - \omega_{\mathbf{p}}a(p)\right]|0\rangle = (\omega_0 - \omega_{\mathbf{p}})a(p)|0\rangle.$$

So,  $a(p)|0\rangle$  is also eigenstate of *H* with the eigenvalue  $\omega_0 - \omega_p$ . This, however, is in contradiction with the fact that  $\omega_0$  is the smallest eigenvalue. The only way how to resolve this contradiction is to assume that  $a(p)|0\rangle = 0$ , for all *p*.

In order to see how to construct *excited states* in our theory, we use the relation

$$[H, a^{\dagger}(p)] = \omega_{\mathbf{p}} a^{\dagger}(p),$$

which implies that

$$Ha^{\dagger}(p)|0\rangle = (\omega_0 + \omega_p)a^{\dagger}(p)|0\rangle,$$

and more generally

$$H[a^{\dagger}(p)]^{n}|0\rangle = (\omega_{0} + n\omega_{p})[a^{\dagger}(p)]^{n}|0\rangle,$$
  

$$H\{[a^{\dagger}(p_{1})]^{n_{1}}[a^{\dagger}(p_{2})]^{n_{2}}...\}|0\rangle$$
  

$$= (\omega_{0} + n_{1}\omega_{p_{1}} + n_{2}\omega_{p_{2}} + ...)\{[a^{\dagger}(p_{1})]^{n_{1}}[a^{\dagger}(p_{2})]^{n_{2}}...\}|0\rangle.$$

This shows that states  $\prod_i [a^{\dagger}(p_i)]^{n_i} |0\rangle$  correspond to excited states with the energy eigenvalue  $(\omega_0 + \sum_i n_i \omega_{p_i})$ . In addition, there are no other states than those created via application of  $a^{\dagger}$  on the vacuum state. If this would not be the case, we could, in contrast assume that there is an exited state  $|\alpha_k\rangle$  such that

$$H|\alpha_k\rangle = (\omega_0 + n_1\omega_{\boldsymbol{p}_1} + n_2\omega_{\boldsymbol{p}_2} + \ldots + \alpha_k\omega_{\boldsymbol{p}_k} + \ldots)|\alpha_k\rangle,$$

where  $\alpha_k$  is not a positive integer. By employing the identity

$$Ha(p)|0\rangle = a(p)H - \omega_p a(p),$$

we would obtain that

$$Ha^{n}(p_{k})|\alpha_{k}\rangle = \left[\omega_{0} + n_{1}\omega_{p_{1}} + \ldots + (\alpha_{k} - n)\omega_{p_{k}} + \ldots\right]a^{n}(p_{k})|\alpha_{k}\rangle$$

This equation implies that also the state  $a^n(p_k)|\alpha_k\rangle$  is an eigenstate of the Hamiltonian. On the other hand, since this is true for any positive integer *n*, we can always choose a sufficiently large *n* that will ensure that the ensuing eigenvalue of  $a^n(p_k)|\alpha_k\rangle$  is negative. This cannot be, however, right since *H* is positive definite operator. The only way out of this paradox is that  $\alpha_k$  is a positive integer.

Typical states are:

►  $|p\rangle = a^{\dagger}(p)|0\rangle$  — *single-particle state*, it creates excitation with energy  $\omega_p$  and momenta p.

In linear harmonic oscillator,  $|1\rangle = a^{\dagger} |0\rangle$  creates excited state with energy  $\omega$  — here no momentum is included, thus one cannot really speak about particle.

|*p*<sub>1</sub>, *p*<sub>2</sub>⟩ = *a*<sup>†</sup>(*p*<sub>1</sub>)*a*<sup>†</sup>(*p*<sub>2</sub>) |0⟩ — *two-particle state*, it creates two excitations, one with energy ω<sub>*p*<sub>1</sub></sub> and momenta *p*<sub>1</sub>, second with energy ω<sub>*p*<sub>2</sub></sub> and momenta *p*<sub>2</sub>.

In linear harmonic oscillator,

$$|2\rangle = \frac{a^{\dagger}a^{\dagger}}{\sqrt{2}}|0\rangle , \qquad (2.139)$$

creates 2 excited states above  $|0\rangle$  with energy  $\omega + \omega = 2\omega$ .

► *Three and higher particle states* can be constructed in the same way.

We can construct a particle number operator

Clearly an analogue of the *energy-level operator* in linear harmonic oscillator. There  $N = a^{\dagger}a$ .

$$N = \int \frac{d^3 p}{(2\pi)^3 2\omega_p} a^{\dagger}(p) a(p) = \sum_{p} a^{\dagger}(p) a(p) , \qquad (2.140)$$

which satisfies

$$[N, a^{\dagger}(p)] = \sum_{p} [a^{\dagger}(p')a(p'), a^{\dagger}(p)]$$
  
= 
$$\sum_{p} a^{\dagger}(p') \underbrace{[a(p'), a^{\dagger}(p')]}_{\delta_{pp'}} = a^{\dagger}(p). \quad (2.141)$$

So, that

$$Na^{\dagger}(p) = a^{\dagger}N + a^{\dagger}(p) = a^{\dagger}(p)(N+1).$$
 (2.142)

Operator *N* thus counts particles (or excitations) in a given state. Indeed, for instance

$$N |0\rangle = \sum_{p} a^{\dagger}(p) a(p) |0\rangle = 0,$$
 (2.143)

so for vacuum, N = 0. Similarly,

$$N |p\rangle = N a^{\dagger}(p) |0\rangle = a^{\dagger}(p)(N+1) |0\rangle = a^{\dagger}(p) |0\rangle = |p\rangle$$
, (2.144)

 $|p\rangle$  is an eigenstate of *N* with *N* = 1. Analogously

$$N |p_1, p_2\rangle = N a^{\dagger}(p_1) a^{\dagger}(p_2) |0\rangle = a^{\dagger}(p_1)(N+1) a^{\dagger}(p_2) |0\rangle$$
  
=  $a^{\dagger}(p_1) a^{\dagger}(p_2)(N+2) |0\rangle = 2 |p_1, p_2\rangle$ , (2.145)

 $|p_1p_2\rangle$  is a 2-particle eigenstate of *N* and similarly for higher excited states. Similarly we could proceed to higher particle states.

#### Note on vacuum energy

In the Hamiltonian (2.135) we have seen that

$$\frac{1}{2} \left( a(p) a^{\dagger}(p) + a^{\dagger}(p) a(p) \right) \; = \; a^{\dagger}(p) a(p) \; + \; \frac{1}{2} \delta_{pp} \; .$$

Since  $\delta_{pp} = (2\pi^3) 2\omega_p \delta(\mathbf{0})$ , we can observe that the (momentum) density of the ground state energy diverges. To understand the structure of this divergence let us first realize that

$$(2\pi)^{3}\delta(0) = \int d^{3}x e^{\pm ipx}|_{p=0} = \int d^{3}x = V,$$

this diverges is in the infinite volume limit. Then,

$$\frac{1}{2}\delta_{pp} = \text{energy density} \cdot V,$$

which implies that the ground state energy reads

$$E_0 = \frac{1}{2} \sum_{p} \omega_p \delta_{pp'}$$
$$= \frac{1}{2} \int \frac{\mathrm{d}^3 p}{(2\pi)^3 2\omega_p} \omega_p (2\pi)^3 2\omega_p \delta(0)$$
$$= \frac{1}{2} \int \frac{\mathrm{d}^3 p}{(2\pi)^3} \omega_p V.$$

Here  $\omega_p V$  is the density of energy with given p in the entire space. This is divergent because for each frequency (momentum) there are infinitely many particles whose number is proportional to the volume of the space. Because the divergent factor V is related to small momenta, the corresponding divergence is called *infrared* or *IR divergence*.

Naively one could assume that the density of the ground state energy could be finite. Unfortunately even this quantity is divergent:

$$\lim_{V \to \infty} \frac{E_0}{V} = \frac{1}{2} \int \frac{\mathrm{d}^3 \boldsymbol{p}}{(2\pi)^3} \omega_{\boldsymbol{p}} = \infty$$

So, the vacuum energy density diverges at  $|\mathbf{p}| \rightarrow \infty$ . This so-called *UV divergence* arises because the "oscillators" with large momentum have very large zero-point energy  $1/2\omega_p \approx |\mathbf{p}|/2$ .

Let us now compare the ground state issue with the one in the linear harmonic oscillator (LHO):

- ► LHO
  - $\omega$  is *p* independent no IR divergence
  - there is only 1 or finite number of oscillators in volume *V* — no IR divergence
- ► QFT
  - frequency ω<sub>p</sub> depends on *p* which changes smoothly over ℝ<sup>3</sup>. For large |*p*| we have that ω<sub>p</sub> ≈ |*p*|,— UV divergence
  - in a given volume *V*, there is infinity of oscillators with different frequencies IR divergence

Typically one wishes to ensure that vacuum has 0 energy and momentum. So, we subtract the ground state energy and define the Hamiltonian to be original Hamiltonian minus ground state energy. We wish to set  $P^{\mu} = \sum_{p} p^{\mu} a^{\dagger}(p) a(p)$ . Now  $P^{\mu} |0\rangle = 0$ .

$$P^{\mu} |p\rangle = \sum_{p'} p^{\mu'} a^{\dagger}(p') a(p') a^{\dagger}(p) |0\rangle = \sum_{p'} p^{\mu'} \left[ a^{\dagger}(p') a(p'), a^{\dagger}(p) \right] |0\rangle$$
  
$$= \sum_{p'} p^{\mu'} a^{\dagger}(p') \left[ a(p'), a^{\dagger}(p) \right] |0\rangle = \sum_{p'} p^{\mu'} a^{\dagger}(p') \delta_{p'p} |0\rangle$$
  
$$= p^{\mu} a^{\dagger}(p) |0\rangle = p^{\mu} |p\rangle. \qquad (2.147)$$

This means that  $|p\rangle$  is an eigenstate of  $P^{\mu}$  with eigenvalue  $p^{\mu}$ .

Vacuum energy is relevant only for the gravitational field. If we neglect gravity then the presence of vacuum energy cannot be detected in usual experiments that are based only on transformations between excited states.

This change does not destroy the significance of the previous calculations with  $p^{\mu}$ , since only commutators were involved. Adjustment by a c-number does not affect commutators.

The subtraction of the vacuum energy does not, however, remove the vacuum fluctuations of the quantum field. This can be evaluated from the so-called *correlation function* 

$$\langle 0 | \phi(\mathbf{x}; t) \phi(\mathbf{y}; t) | 0 \rangle. \qquad (2.146)$$

Similarly as subtraction of vacuum energy in LHO does not remove fluctuation in p or x.

For two particle states:

$$P^{\mu} |p_{1}, p_{2}\rangle = \sum_{p'} p^{\mu'} (a^{\dagger}(p')a(p')a^{\dagger}(p_{1})a^{\dagger}(p_{2}) |0\rangle$$

$$= \sum_{p'} p^{\mu'} \left[ a^{\dagger}(p')a(p'), a^{\dagger}(p_{1})a^{\dagger}(p_{2}) \right] |0\rangle$$

$$= \sum_{p'} p^{\mu'}a^{\dagger}(p') \left[ a(p'), a^{\dagger}(p_{1})a^{\dagger}(p_{2}) \right] |0\rangle$$

$$= \sum_{P'} p^{\mu'}a^{\dagger}(p') \left[ a^{\dagger}(p_{2})\delta_{p'p_{1}} + a^{\dagger}(p_{1})\delta_{pp_{2}} \right] |0\rangle$$

$$= (p_{1}^{\mu} + p_{2}^{\mu})a^{\dagger}(p_{1})a^{\dagger}(p_{2}) |0\rangle$$

$$= (p_{1}^{\mu} + p_{2}^{\mu}) |p_{1}, p_{2}\rangle. \qquad (2.148)$$

This means that  $|p_1, p_2\rangle$  is an eigenstate of  $P^{\mu}$  with  $(p_1^{\mu} + p_2^{\mu})$  as eigenvalue. Etc. for higher particle states. This once more justify the usage of the particle picture description.

#### Occupation number representation — 1st bite

In case we have  $n_{p_1}$  particles with the momenta  $p_1$ ,  $n_{p_2}$  particles with the momenta  $p_2$ , etc., it is customary to write the corresponding  $\sum_i n_{p_i}$ -particle state as

Compare with LHO *n*-th excited state:

$$|n\rangle \; = \; \frac{(a^\dagger)^n}{\sqrt{n}!} \; |0\rangle \; . \label{eq:nlambda}$$

$$|n_{p_1}, n_{p_2}, \cdots \rangle \equiv |\{n_p\}\rangle = \frac{(a_{p_1}^{\dagger})^{n_{p_1}}}{\sqrt{n_{p_1}!}} \frac{(a_{p_2}^{\dagger})^{n_{p_2}}}{\sqrt{n_{p_2}!}} \cdots |0\rangle .$$

This way of representing momentum eigenstates of free fields is known as the occupation number representation. For instance, in the occupation number representation we would have for a 2-particle state

$$|p_i, p_j\rangle = |\underbrace{0}_{p_1} \underbrace{0}_{p_2} \dots \underbrace{1}_{p_i} \dots \underbrace{0}_{p_j} \dots \underbrace{1}_{p_j} \dots \langle 2.149\rangle$$
(2.149)

- occupation number representation takes into account automatically symmetric exchange of particles (bosonic indistinguishability) as no labeling of particles is present in the state description,
- ► occupation number basis is an orthonormal basis on the Hilbert space  $\mathcal{H}_N$  for each fixed  $N = \sum_i n_{p_i}$ ,
- ► normalization to 1 is intuitive  $\langle n_{p_1} \dots n_{p_k} \dots | n'_{p_1} \dots n'_{p_k} \dots \rangle = 1$ , only when n' = n for all  $p_i$ .

The Hilbert space can be combined in the so called *Fock space* 

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \dots = \bigoplus_{N=0}^{\infty} \mathcal{H}_N \equiv \sum_{N=0}^{\infty} \oplus \mathcal{H}_N.$$

Here, the Hilbert space  $\mathcal{H}_0$  only contains one element, the vacuum  $|0\rangle = |0, 0, 0, \dots 0 \dots \rangle$ .

Note that because [N, H] = 0, we can place ourselves in the *N*-particle sector and stay there. This is, of course, the characteristic property of a free theory. Since, interactions generally *create* and *destroy* particles,

they allow to move between different particle sectors of the Fock space.

# 2.5 Normal ordered product

The zero-point energy can be removed automatically by interpreting product of field operators (from classical formulas) as the so-called *normal ordered product*.

To see what is involved, we recall that scalar field can be written as  $\phi = \phi^+(x) + \phi^-(x)$  with  $\phi^+(x) = \sum_{\mathbf{P}} a(p)e^{-ipx}$  being positive frequency part and  $\phi^-(x) = \sum_{\mathbf{P}} a^{\dagger}(p)e^{ipx}$  negative frequency part. That provides

$$\phi(x)\phi(y) = (\phi^+ + \phi^-)_x(\phi^+ + \phi^-)_y$$
  
=  $\phi^+_x \phi^+_y + \phi^-_x \phi^-_y + \phi^-_x \phi^+_y + \phi^+_x \phi^-_y.$  (2.150)

Normal ordering is defined as

$$: \phi(x)\phi(y) := \phi^{+}(x)\phi^{+}(y) + \phi^{-}(x)\phi^{+}(y) + \phi^{-}(y)\phi^{+}(x) + \phi^{-}(x)\phi^{-}(y).$$
(2.151)

The key point in this relation is that  $\langle 0|: \phi(x)\phi(y): |0\rangle = 0$ . Because  $\phi^+(x)\phi^-(y)$  and  $\phi^-(y)\phi^+(x)$  differ only by *c*-number and because  $\langle 0|c$ -number $|0\rangle = c$ -number, we get

$$: \phi(x)\phi(y) := \phi(x)\phi(y) - \langle 0| \phi(x)\phi(y) | 0 \rangle .$$
 (2.152)

So, in :  $\cdots$  : we move all  $\phi^+$ 's to the right and all  $\phi^-$ 's to the left. Having use of this notation we can write

$$P^{\mu} = \int d^3 \mathbf{x} : T^{0\mu} : . \qquad (2.153)$$

Here :  $T^{\mu\nu}(x)$  : is defined as

$$: T^{\mu\nu}(x) := :\partial^{\mu}\psi(x)\partial^{\nu}\psi(x) : -\eta^{\mu\nu} : \mathcal{L}(x) :, \qquad (2.154)$$

so, in particular

$$P^{\mu} = \frac{1}{2} \sum_{p} p^{\mu} : a(p)a^{\dagger}(p) + a^{\dagger}(p)a(p) := \sum_{p} p^{\mu}a_{p}^{\dagger}a_{p} .$$
(2.155)

Note that for  $p^i$  normal ordering is not needed since  $\sum_{p} \frac{p^i}{2} = 0$ .

#### Note on normal ordering

Difference between the Hamiltonian defined via (2.155) and the one with vacuum-energy contribution can be viewed as an ordering ambiguity in moving from the classical to quantum theory.

For instance, we could defined the classical Hamiltonian of the

Linear Harmonic Oscillator as

$$H = \frac{1}{2}(\omega q - ip)(\omega q + ip),$$

which is the same as the conventional choice. At this stage we could promote this *H* to an operator (preserving a given classical ordering) and define the ladder operators as in (2.28). Upon quantization this would give

 $H = \omega a^{\dagger} a.$ 

This part is somehow out of lecture's main line of development and may be omitted in a first reading.

Let us mention, in connection with the energy-momentum tensor, that there exists a simple prescription for a computation of  $T^{\mu\nu}$  that is inspired by general relativity. This prescription gives, by its very definition, the energy-momentum tensor that is symmetric and in usual cases coincides with  $T^{\mu\nu}$  that is obtained via Noether theorem (see Chapter 3). This, so-called *Hilbert energy-momentum tensor* is defined as

$$T_{\mu\nu} = \frac{2}{\sqrt{-g}} \frac{\delta S}{\delta g^{\mu\nu}}, \qquad (2.156)$$

where  $g = \det(g_{\mu\nu})$ . (2.157) is explicitly symmetric and, in addition, covariantly conserved  $D_{\mu}T^{\mu\nu} = 0$  ( $D_{\mu}$  is the so-called covariant derivative). In the Minkowski spacetime  $D_{\mu}T^{\mu\nu} \rightarrow \partial_{\mu}T$ .

To see, that this prescription yields (2.106) let us apply it to our scalarfield situation. So, we first formulate the Lagrangian with a generic metric tensor  $g^{\mu\nu}$  and at the end of computations we set  $g^{\mu\nu}$  to  $\eta^{\mu\nu}$ . We first recall that

$$\frac{\delta S[g,\phi]}{\delta g^{\mu\nu}(y)} = \left. \frac{\mathrm{d} S[g+\epsilon\delta(\cdot-y)]}{\mathrm{d}\epsilon^{\mu\nu}} \right|_{\epsilon=0},\tag{2.157}$$

which implies that

$$2\frac{\delta S[g,\phi]}{\delta g^{\mu\nu}(y)} = \int d^4x \left[ \frac{\delta \sqrt{-g(x)}}{\delta g^{\mu\nu}(y)} \left( g^{\alpha\beta} \partial_\alpha \phi \partial_\beta \phi - m^2 \phi^2 \right) \right. \\ \left. + \sqrt{-g} \frac{\delta g^{\alpha\beta}(x)}{\delta g^{\mu\nu}(y)} \partial_\alpha \phi \partial_\beta \phi \right].$$
(2.158)

The first functional derivative on the RHS can be computed as fol-

lows

$$\frac{\delta\sqrt{-g(x)}}{\delta g^{\mu\nu}(y)} = \frac{\delta\sqrt{-\det g_{\mu\nu}(x)}}{\delta g^{\mu\nu}(y)} = \frac{\delta\left(1/\sqrt{-\det g^{\mu\nu}(x)}\right)}{\delta g^{\mu\nu}(y)}$$

$$= \frac{1}{2}\frac{1}{\sqrt{-\det g^{\mu\nu}}}\frac{1}{d\epsilon^{\mu\nu}}\frac{d}{d\epsilon^{\mu\nu}}\det(g^{\mu\nu}(x) + \epsilon^{\mu\nu}\delta(x-y))\Big|_{\epsilon=0}$$

$$= \frac{1}{2}\sqrt{-g}\frac{d}{d\epsilon^{\mu\nu}}e^{\operatorname{Tr}[\det(g^{\mu\nu}(x) + \epsilon^{\mu\nu}\delta(x-y))]}\Big|_{\epsilon=0}$$

$$= -\frac{1}{2}\sqrt{-g}\frac{d}{d\epsilon^{\mu\nu}}e^{\operatorname{Tr}\left[\det\left(\delta^{\alpha}_{\beta}(x) + \epsilon^{\alpha\gamma}g_{\gamma\beta}\delta(x-y)\right)\right]}\Big|_{\epsilon=0}$$

$$= -\frac{1}{2}\sqrt{-g}\frac{d}{d\epsilon^{\mu\nu}}e^{\epsilon^{\alpha\gamma}g_{\gamma\alpha}\delta(x-y)}\Big|_{\epsilon=0}$$

$$= -\frac{1}{2}\sqrt{-g}g_{\mu\nu}\delta(x-y). \qquad (2.159)$$

Here we used the fact that for any matrix *A* the following identity holds:

$$\det A = e^{\operatorname{Tr}(\log A)}.$$

The second functional derivative on the RHS of (2.158) reads

$$\frac{\delta g^{\alpha\beta}(x)}{\delta g^{\mu\nu}(y)} = \frac{\mathrm{d}}{\mathrm{d}\epsilon^{\mu\nu}} \left[ g^{\alpha\beta}(x) + \epsilon^{\alpha\beta}\delta(x-y) \right] = \delta^{\alpha}_{\mu}\delta^{\beta}_{\nu}\delta(x-y) \,. \tag{2.160}$$

Combining the previous two results with (2.157) and (2.158) we obtain

$$T^{\mu\nu}(y) = \left[ -\frac{1}{2} g^{\mu\nu} \left( g_{\alpha\beta} \partial^{\alpha} \phi(y) \partial^{\beta} \phi(y) - m^{2} \phi^{2}(y) \right) + \partial^{\mu} \phi(y) \partial^{\nu} \phi(y) \right].$$
(2.161)

If we now set  $g^{\mu\nu} = \eta^{\mu\nu}$ , then

$$T^{\mu\nu}(y) = \partial^{\mu}\phi(y)\partial^{\nu}\phi(y) - \eta^{\mu\nu}\mathcal{L}(y).$$
(2.162)

So, in particular

$$T^{00} = \pi \dot{\phi} - \mathcal{L} = \mathcal{H},$$
  

$$T^{0i} = T^{i0} = \pi \partial^{i} \phi = -\pi \nabla_{i} \phi,$$
(2.163)

as it should.

# 2.6 Multiplet of Scalar Fields

Let us now pass from a single scalar field to a multiplet of *n* fields (also known as *n*-tuplet), i.e.,  $\phi(x) \rightarrow \phi(x) = \{\phi_r(x)\}_{r=1}^n$  and  $\phi_r^{\dagger} = \phi_r$  for all fields in the multiplet. Then the corresponding Lagrangian for free multiplet fields can be written in the form

$$\mathcal{L}(\phi_r, \dot{\phi_r}, \nabla \phi_r) = \sum_r \frac{1}{2} (\partial_\mu \phi_r \partial^\mu \phi_r - m^2 \phi_r^2), \qquad (2.164)$$

where we have assumed that all fields have an equal mass:  $m_r = m$ . Again, we can set up the commutation relations. In this case we have

$$\begin{split} & [\phi_r(\mathbf{x}, t), \pi_s(\mathbf{y}, t)] = i \delta_{rs} \delta(\mathbf{x} - \mathbf{y}), \\ & [\phi_r(\mathbf{x}, t), \phi_s(\mathbf{y}, t)] = [\pi_r(\mathbf{x}, t), \pi_s(\mathbf{y}, t)] = 0, \end{split}$$
(2.165)

where

$$\pi_r(\boldsymbol{x},t) = \frac{\delta S[\phi]}{\delta \dot{\phi}_r(\boldsymbol{x},t)} = \frac{\partial \mathcal{L}(\phi(\boldsymbol{x}), \partial_\mu \phi(\boldsymbol{x}))}{\partial \dot{\phi}_r(\boldsymbol{x},t)}.$$
 (2.166)

For Hamiltonian we get

$$H = \sum_{r} \int d^{3}x \,\pi_{r}(x,t) \dot{\phi_{r}}(x,t) - L$$
  
=  $\frac{1}{2} \sum_{r} \int d^{3}x \left[ \pi_{r}^{2}(x,t) + (\nabla \phi_{r}(x,t))^{2} + m^{2} \phi^{2}(x,t) \right].$  (2.167)

By analogy to a single-field case we get the mode expansion

$$\phi_r(x) = \sum_{p} \left( a_r(p) e^{-ipx} + a_r^{\dagger}(p) e^{ipx} \right) , \qquad (2.168)$$

and ensuing commutation relations for mode operators

$$\left[a_r(p), a_s^{\dagger}(p')\right] = \delta_{rs} \delta_{pp'}. \qquad (2.169)$$

Vacuum state  $|0\rangle$  is defined so that

$$a_r(p) |0\rangle = 0,$$
 (2.170)

for all *p* and *r*. After appropriate normal ordering we get

$$\hat{P}^{\mu} = \sum_{p,r} p^{\mu} a_{r}^{\dagger}(p) a_{r}(p) , \qquad (2.171)$$

and the operator of a particle number

Operator  $N_r$  counts only particles of r-th type.

$$\hat{N} = \sum_{r} \hat{N}_{r} = \sum_{p,r} a_{r}^{\dagger}(p) a_{r}(p) \,. \tag{2.172}$$

Eigenstates of  $\hat{N}$  and  $\hat{P}^{\mu}$  are typically of the form

$$a_{r_1}^{\dagger}(p_1)a_{r_2}^{\dagger}(p_2)\dots|0\rangle = |p_1r_1, p_2r_2, \dots\rangle.$$
 (2.173)

Then

$$\hat{P}^{\mu} | p_{1}r_{1}, p_{2}r_{2}, \ldots \rangle = (p_{1} + p_{2} + \ldots)^{\mu} | p_{1}r_{1}, p_{2}r_{2}, \ldots \rangle ,$$

$$\hat{N}_{r} | N_{r_{1}}, N_{r_{2}}, \ldots, N_{r}, \ldots, N_{r_{n}}, \ldots \rangle$$

$$= \sum_{p} n_{r}(p) | N_{r_{1}}, N_{r_{2}}, \ldots, N_{r_{n}}, \ldots \rangle . \quad (2.174)$$

Here  $N_{r_i}$  denotes a set of occupation numbers with identical  $r_i$ , i.e.  $N_{r_i} = \{n_{r_i}(p_1), n_{r_i}(p_2), n_{r_i}(p_3) \dots\}.$ 

# **Special case** n = 2

In this case the multiplet has the form

$$\boldsymbol{\phi}(x) = \begin{pmatrix} \phi_1(x) \\ \phi_2(x) \end{pmatrix}. \tag{2.175}$$

In this connection it is convenient to define associated *complex* or *non-hermitian* fields

$$\phi(x) = \frac{1}{\sqrt{2}} (\phi_1(x) + i\phi_2(x)) ,$$
  
$$\phi^{\dagger}(x) = \frac{1}{\sqrt{2}} (\phi_1(x) - i\phi_2(x)) . \qquad (2.176)$$

The corresponding Lagrangian reads

$$\mathcal{L} = \sum_{r=1}^{2} \left( \frac{1}{2} \partial_{\mu} \phi_r(x) \partial^{\mu} \phi_r(x) - \frac{1}{2} m^2 \phi_r^2(x) \right)$$
$$= \partial_{\mu} \phi^{\dagger}(x) \partial^{\mu} \phi(x) - m^2 \phi^{\dagger}(x) \phi(x) . \qquad (2.177)$$

Canonically conjugate momenta are

$$\pi^{\dagger}(\boldsymbol{x},t) = \frac{\partial \mathcal{L}(\boldsymbol{x})}{\partial \dot{\phi}^{\dagger}(\boldsymbol{x},t)} = \dot{\phi}(\boldsymbol{x},t),$$
  
$$\pi(\boldsymbol{x},t) = \frac{\partial \mathcal{L}(\boldsymbol{x})}{\partial \dot{\phi}(\boldsymbol{x},t)} = \dot{\phi}^{\dagger}(\boldsymbol{x},t). \qquad (2.178)$$

With this we can formulate the Hamilton operator via the Legendre transformation as

$$H = \int d^{3}\mathbf{x} \left[ \pi(\mathbf{x},t)\dot{\phi}(\mathbf{x},t) + \pi^{\dagger}(\mathbf{x},t)\dot{\phi}^{\dagger}(\mathbf{x},t) - \mathcal{L}(\mathbf{x}) \right]$$
  
$$= \int d^{3}\mathbf{x} \left[ \pi(\mathbf{x},t)\pi^{\dagger}(\mathbf{x},t) + \pi^{\dagger}(\mathbf{x},t)\pi(\mathbf{x},t) - \mathcal{L}(\mathbf{x}) \right]$$
  
$$= \int d^{3}\mathbf{x} \left[ \pi^{\dagger}(\mathbf{x},t)\pi(\mathbf{x},t) + \nabla\phi^{\dagger}(\mathbf{x},t)\nabla\phi(\mathbf{x},t) + m^{2}\phi^{\dagger}(\mathbf{x},t)\phi(\mathbf{x},t) \right]. \qquad (2.179)$$

Note that there is no problem with ordering  $\pi^{\dagger}\pi$  versus  $\pi\pi^{\dagger}$  and  $\phi^{\dagger}\phi$  versus  $\phi\phi^{\dagger}$ . This is because the canonical commutation relations acquire the form

$$[\phi(\mathbf{x},t),\pi(\mathbf{y},t)] = i\delta(\mathbf{x}-\mathbf{y}), \quad [\phi^{\dagger}(\mathbf{x},t),\pi^{\dagger}(\mathbf{y},t)] = i\delta(\mathbf{x}-\mathbf{y}),$$
  

$$[\phi(\mathbf{x},t),\phi(\mathbf{y},t),] = [\phi(\mathbf{x},t),\phi^{\dagger}(\mathbf{y},t),]$$
  

$$= [\phi(\mathbf{x},t),\pi^{\dagger}(\mathbf{y},t),] = \text{etc.} = 0.$$
 (2.180)

By having (2.180) at our disposal we can write the Heisenberg evolution equations as

$$\begin{split} \dot{\phi}(\mathbf{x},t) &= i[H,\phi(\mathbf{x},t)] = \pi^{\dagger}(\mathbf{x},t), \\ \dot{\phi}^{\dagger}(\mathbf{x},t) &= i[H,\phi^{\dagger}(\mathbf{x},t)] = \pi(\mathbf{x},t), \\ \dot{\pi}(\mathbf{x},t) &= i[H,\pi(\mathbf{x},t)] = \nabla^{2}\phi^{\dagger}(\mathbf{x},t) - m^{2}\phi^{\dagger}(\mathbf{x},t), \\ \dot{\pi}^{\dagger}(\mathbf{x},t) &= i[H,\pi^{\dagger}(\mathbf{x},t)] = \nabla^{2}\phi(\mathbf{x},t) - m^{2}\phi(\mathbf{x},t). \end{split}$$
(2.181)

These equations are equivalent to two autonomous second-order partial differential equations

$$\ddot{\phi}^{\dagger} - \nabla^2 \phi^{\dagger} + m^2 \phi^{\dagger} = 0 \quad \Leftrightarrow \quad \left(\Box + m^2\right) \phi^{\dagger} = 0 ,$$
  
$$\ddot{\phi} - \nabla^2 \phi + m^2 \phi = 0 \quad \Leftrightarrow \quad \left(\Box + m^2\right) \phi = 0 .$$
(2.182)

From these equations we get the solution in terms of plane wave mode expansion

Note that since the fields are nonhermitian we have that  $b \neq a$ .

$$\phi(x) = \sum_{p} \left[ a(p)e^{-ipx} + b^{\dagger}(p)e^{ipx} \right],$$
  
$$\phi^{\dagger}(x) = \sum_{p} \left[ b(p)e^{-ipx} + a^{\dagger}(p)e^{ipx} \right].$$
 (2.183)

In order to reproduce the canonical commutation relations for fields, we need that the mode operators satisfy

$$[a(p), a^{\dagger}(p')] = \delta_{pp'} = [b(p), b^{\dagger}(p')],$$
  
$$[a(p), a(p')] = [b(p), b(p')] = [a(p), b(p')] = \text{etc.} = 0. \quad (2.184)$$

After normal ordering we have

$$\hat{P}^{\mu} = \sum_{p} p^{\mu} \left[ a^{\dagger}(p)a(p) + b^{\dagger}(p)b(p) \right] .$$
(2.185)

Corresponding eigenstates of  $\hat{P}^{\mu}$  are  $|0\rangle$ ,  $a^{\dagger}(p)|0\rangle$ ,  $b^{\dagger}(p)|0\rangle$ , etc., where the vacuum state  $|0\rangle$  is defined so that

$$a(p)|0\rangle = b(p)|0\rangle = 0, \qquad (2.186)$$

for all *p*. So, for instance,

$$\hat{P}^{\mu}|p_{1}, p_{2}, \dots, q_{1}, q_{2} \dots\rangle = \hat{P}^{\mu}a^{\dagger}(p_{1})a^{\dagger}(p_{2})\cdots b^{\dagger}(q_{1})b^{\dagger}(q_{2})\cdots|0\rangle$$
$$= (p_{1}+p_{2}+\dots+q_{1}+q_{2}+\dots)^{\mu}|p_{1}, p_{2}, \dots, q_{1}, q_{2}\dots\rangle. \quad (2.187)$$

We can also define operators that count number of particles of *a*- and *b*-type as

$$\hat{N}_a = \sum_{p} a^{\dagger}(p) a(p), \quad \hat{N}_b = \sum_{p} b^{\dagger}(p) b(p).$$
 (2.188)

#### **Conserved current**

The complex scalar field is associated with a *conserved current*. Actual existence and form of such a current will be deduced from *Noether's theorem* in Chapter 2.9.

Let us now state (without proof) that the conserved current has the form

$$J^{\mu}(x) = i \left[ \phi^{\dagger}(x) \partial^{\mu} \phi(x) - (\partial^{\mu} \phi^{\dagger}(x)) \phi(x) \right].$$
(2.189)

It is easy to see that Heisenberg's equations of motion imply that  $\partial_{\mu}J^{\mu}(x) = 0$ , indeed

$$\partial_{\mu}J^{\mu} = \left(i\partial_{\mu}\phi^{\dagger}\partial^{\mu}\phi + i\phi^{\dagger}\Box\phi - i(\Box\phi^{\dagger})\phi - i\partial^{\mu}\phi^{\dagger}\partial_{\mu}\phi\right)$$
$$= i\phi^{\dagger}\Box\phi - i(\Box\phi^{\dagger})\phi = -im^{2}\phi^{\dagger}\phi + im^{2}\phi^{\dagger}\phi = 0. \quad (2.190)$$

In addition, we can define the *charge* as

$$Q = \int d^3 \mathbf{x} J^0(x) = \int dV n_{\mu} J^{\mu}(x) \,. \tag{2.191}$$

Here  $n_{\mu}$  is unite timelike vector and dV is a volume element of a 3dimensional hypersurface orthogonal to  $n_{\mu}$ . This charge is not only Lorentz scalar, i.e.  $Q(n) = Q(L^{-1}n)$  (proof is the same as in Chapter 1.3) but, most importantly, it is conserved. This can be seen most easily by rewriting Q in terms of mode operators. On substituting the mode expansion of fields to Q we get (after normal ordering)

$$Q = \sum_{p} \left[ a^{\dagger}(p)a(p) - b^{\dagger}(p)b(p) \right] = \hat{N}_{a} - \hat{N}_{b} .$$
 (2.192)

By emplying now the form of  $H = \hat{P}^0$  from (2.185) together with commutation relations (2.184) we immediately get that

$$[H,Q] = \sum_{p,p'} \{ [a^{\dagger}(p)a(p), a^{\dagger}(p')a(p')] - [b^{\dagger}(p)b(p), b^{\dagger}(p')b(p')] \}$$
  
= 0. (2.193)

From the explicit form (2.228) we see that

$$Q|0\rangle = 0,$$
  

$$Q|p\rangle_{a} = Qa^{\dagger}(p)|0\rangle = \sum_{p} [a^{\dagger}(p')a(p'), a^{\dagger}(p)]|0\rangle$$
  

$$= a^{\dagger}(p)|0\rangle = |p\rangle_{a}.$$
(2.194)

General action of Q operator on states generated by creation operators  $a^{\dagger}$  (*a*-type particle states) can be deduced from the simple algebraic fact that

$$Qa^{\dagger}(p) = a^{\dagger}(p)(Q+1)$$
. (2.195)

Indeed, consider, e.g., state  $|p_1, p_2\rangle$  then

$$Q|p_1, p_2\rangle_a = Qa^{\dagger}(p_1)a^{\dagger}(p_2)|0\rangle = a^{\dagger}(p_1)a^{\dagger}(p_2)(Q+2)|0\rangle$$
  
= 2|p\_1, p\_2\rangle\_a. (2.196)

For a generic *n* (*a*-type) particle state

$$Q|p_1, p_2, ... \rangle_a = \hat{N}_a |p_1, p_2, ... \rangle_a = n |p_1, p_2, ... \rangle_a.$$
(2.197)

Similarly, for *b*-type particle states we can write (using the identity  $Qb^{\dagger}(p) = b^{\dagger}(p)(Q-1)$ )

$$Qb^{\dagger}(q)|0\rangle = Q|q\rangle_{b} = b^{\dagger}(q)(Q-1)|0\rangle$$
$$= -b^{\dagger}(q)|0\rangle = -|q\rangle_{b}, \qquad (2.198)$$

and generally for n' (*b*-type) particle state

$$Q|q_1, q_2, \ldots\rangle_b = -\hat{N}_b |q_1, q_2, \ldots\rangle_b = -n' |q_1, q_2, \ldots\rangle_b.$$
(2.199)

Finally, when we act with *Q* on states having *n a*-type particles and *n*' *b*-type particles we get

$$Q|p_{1}, p_{2}, \dots, q_{1}, q_{2} \dots\rangle = Qa^{\dagger}(p_{1})a^{\dagger}(p_{2}) \cdots b^{\dagger}(q_{1})b^{\dagger}(q_{2}) \cdots |0\rangle$$
  
=  $a^{\dagger}(p_{1}) \cdots b^{\dagger}(q_{1}) \cdots (Q + n - n')|0\rangle$   
=  $(n - n')|p_{1}, p_{2}, \dots, q_{1}, q_{2} \dots\rangle.$  (2.200)

We thus see that the charge Q associates with each particle of *a*-type a positive conserved quantity (of unit norm), while with each *b*-type particle a negative quantity (of unit norm). This is reminiscent of the concept of electric charge (in appropriately measured units). One could formally call particles *a* as positrons and particles *b* as electrons. At present we have no justification for this picture even though the name *charge* evokes the electric charge. In quantum theory and analytical mechanics the name *charge* has more general meaning — it is a time conserved quantity that is deduced from symmetry principles. Proper terminology is *Noether charge* and we will have more to say about this in Chapter 2.9.

# 2.7 Fock space and occupation number representation — another bite

In QM *n*-particle state contains clear information about which particle occupies which one-particle state. This is unphysical due to the indistinguishability of particles. In order to accommodate *identical particles* one has to construct symmetric (or asymmetric) *n*-particle state. In such a case information about *which particle occupies which one-particle state* is eliminated, and the only information which remains is how many particles, say  $n_r$ , occupy a given single-particle state, say  $|v_r\rangle$ . These many-particle wavefunctions are rather cumbersome to work with in

On the other hand, for our specific dynamical system the charge Q can be, indeed, in many cases identified with a *total electric charge* since it is associated with a symmetry U(1) that is a key symmetry in theory of electromagnetism.

By *identical* we mean that all intrinsic physical properties of the particles are the same — indistinguishable. For example, all electrons are identical since they have the same rest mass, electric charge, and spin. practice. It is often more convenient (and in Quantum Field Theory customary) to use an alternative (though equivalent) formalism. This formalism is phrased directly in terms of the *occupation numbers* of single-particle states.

To understand what is involved, let us review some fundamentals from many-body quantum mechanics. To this end we consider the (normalized) set of wave functions  $|v\rangle$  of a single-particle Hamiltonian, i.e.,  $\hat{h}|v\rangle = E_{v}|v\rangle$ . With this notation the normalized two-particle state of two bosons occupying energy levels  $v_1$  and  $v_2$  is given by the symmetrized product

$$\psi^{(S)}(x_1, x_2) = \frac{1}{\sqrt{2}} \left( \langle x_1 | \nu_1 \rangle \langle x_2 | \nu_2 \rangle + \langle x_1 | \nu_2 \rangle \langle x_2 | \nu_1 \rangle \right)$$
$$= \left( \langle x_1 | \otimes \langle x_2 | \rangle | \nu_1, \nu_2 \rangle, \qquad (2.201) \right)$$

where the ket state  $|v_1, v_2\rangle$  has the explicit form

$$|\nu_1, \nu_2\rangle = \frac{1}{\sqrt{2}} (|\nu_1\rangle \otimes |\nu_2\rangle + |\nu_2\rangle \otimes |\nu_1\rangle) .$$
 (2.202)

Strictly speaking, state  $\psi^{(S)}(x_1, x_2)$  is an eigenstate of the Hamiltonian  $\hat{H} = \hat{h}(x_1) + \hat{h}(x_2)$ .

In the *n*-body problem the Hamiltonian has a typical structure  $\hat{H} = \hat{H}_0 + \hat{H}_I$ , where

$$\hat{H}_0 = \sum_{i=1}^n \hat{h}(x_1), \qquad (2.203)$$

is a *single-particle operator* (i.e.,  $H_0$  is a sum of terms, each involving the coordinates of only one particle), while  $H_I$  is a *multi-particle operator* (i.e., it is a sum of terms each involving the coordinates of more than one particle). In the perturbation treatment one considers  $H_I$  as being in some sense small. The objective of the perturbation theory is then to express the energy spectrum and eigenstates of H in terms of the energy levels and eigenstates of  $H_0$ . The corresponding *n*-particle eigenstates of  $H_0$  are given by the symmetrized product

$$|v_1,\ldots,v_n\rangle = \frac{1}{\sqrt{n!\Pi_{\nu}(n_{\nu})!}} \sum_{\pi \in S_n} |v_{\pi_1}\rangle \otimes |v_{\pi_2}\rangle \otimes \cdots \otimes |v_{\pi_n}\rangle$$
, (2.204)

where the summation is over all permutations that belong to the permutation group  $S_n$ . The prefactor  $1/\sqrt{n!\Pi_v(n_v)!}$  ensures the normalization of wave function  $|v_1, \ldots, v_n\rangle$  to 1. For fermions we would need to consider antisymmetrized product of single-particle states, namely

$$|\nu_1,\ldots,\nu_n\rangle = \frac{1}{\sqrt{n!}} \sum_{\pi \in S_n} (-1)^{(1-\operatorname{sgn}\pi)/2} \left( |\nu_{\pi_1}\rangle \otimes |\nu_{\pi_2}\rangle \otimes \cdots \otimes |\nu_{\pi_n}\rangle \right).$$
(2.205)

Here sgn  $\pi = 1$  (or -1) if the permutations are even (or odd). The *n*-particle wave functions (2.205) are known as *Slater determinants*.

Formulation of *n*-body particle wave functions in terms of symmetrized

 $n_{\nu}$  represents a total number of particles in state  $\nu$ , i.e.,  $\sum_{\nu} n_{\nu} = n$ .

Because the occupation number  $n_{\nu}$  for fermions is ether 0 or 1, the would be factor  $\Pi_{\nu}(n_{\nu})! = 1$ .

or antisymmetrized products of single-particle states is not very convenient in QFT. Here we state some reasons.

- Practical computations in the language of base vectors (2.204) or (2.205) are very cumbersome. E.g., in order to compute the overlap of two *n*-body wavefunctions one needs to form (*n*!)<sup>2</sup> scalar products.
- ▶ Representation in terms of (2.204) or (2.205) is tailor-made for problems with fixed number of particles. But that is not the case in relativistic QFT. Even in non-relativistic QFT where the number of particles is fixed but *n* is very large (e.g. in solid-state physics a typical scale is  $n \sim 10^{23}$ ) it is known from statistical mechanics that it is technically more convenient to work in grand-canonical ensemble approach (rather than canonical one) where *n* is not fixed.
- ► Typical question one asks in QFT is, "What is the probability amplitude (or probability) that a particle produced at a certain space-time point x<sub>1</sub><sup>µ</sup> will be annihilated (will decay) at some other space-time point x<sub>2</sub><sup>µ</sup>?" These types of questions can be better addressed in representations, which are directly phrased in terms of occupation numbers of individual particles rather than the entangled set of quantum numbers of all constituents.

To find more suitable representation for wave functions let us order  $v_i$  in the ascending sense, e.g., when  $v_i = p_i$  ( $p_i$  are moments) then

$$|p_1, p_2..., p_n\rangle$$
, where  $p_1 \le p_2 \le p_3 \le \cdots \le p_n$ . (2.206)

So, for instance, the state

$$|p_1, p_1, p_1, p_2, p_2, p_3, p_3, p_3, p_4, p_5, p_6 \dots \rangle$$
, (2.207)

contains a redundancy and a more efficient encoding of the state might read

$$|3p_1, 2p_2, 3p_3, 1p_4, 1p_5, 1p_6, \ldots\rangle$$
 or  $|3, 2, 3, 1, 1, 1, \ldots\rangle$ . (2.208)

We will more abstractly denote such states as  $|\{n_p\}\rangle$ , where  $\{n_p\}$  is set of occupation numbers, e.g., in (2.244)  $\{n_p\} = 3, 2, 3, 1, 1, 1, ...$  States  $|\{n_p\}\rangle$  are known as *occupation number representation* states.

Recall that for free Klein-Gordon field the Hamiltonian has the form

$$H = \sum_{p} \omega_{p} a^{\dagger}(p) a(p) = \sum_{p} \omega_{p} a_{p}^{\dagger} a_{p}. \qquad (2.209)$$

This is has the structure of the single-particle operator  $\hat{H}_0$  in (2.203) with  $\hat{h}(p) = \omega_p a_p^{\dagger} a_p$ . This, in turn, implies that states like (2.207) must be eigenstates of *H*.

Let us now observe that the free Hamiltonian *H* commutes with the total particle-number operator  $N = \sum_{k} a_{k}^{\dagger} a_{k} = \sum_{k} \hat{n}_{k} (\hat{n}_{k} = a_{k}^{\dagger} a_{k} \text{ determines how many particles occupy the state$ *k* $}. In addition, also$ 

For 4-momenta the ascending order is meant is the sense of vector ordering, e.g., 4-vectors with bigger 0th component are more to the right, if 0th components are identical then 4-vectors with bigger 1st component are positioned more to the right, etc.

Corresponding single-particle states are denoted not only by  $\omega_p$  but also by p because the momentum operator commutes with  $\hat{h}(p)$ .

 $N, \hat{n}_k, \hat{n}_{k'}$  commute pairwise. For instance

$$\begin{bmatrix} \hat{n}_{k}, \hat{n}_{k'} \end{bmatrix} = \begin{bmatrix} a_{k}^{\dagger} a_{k}, a_{k'}^{\dagger} a_{k'} \end{bmatrix} = a_{k}^{\dagger} \begin{bmatrix} a_{k}, a_{k'}^{\dagger} a_{k'} \end{bmatrix} + \begin{bmatrix} a_{k}^{\dagger}, a_{k'}^{\dagger} a_{k'} \end{bmatrix} a_{k}^{\dagger}$$
$$= a_{k}^{\dagger} \begin{bmatrix} a_{k}, a_{k'}^{\dagger} \end{bmatrix} a_{k'} + a_{k'}^{\dagger} \begin{bmatrix} a_{k}^{\dagger}, a_{k'} \end{bmatrix} a_{k} = 0$$
(2.210)

In this derivation we have used  $\left[a_{k}, a_{k'}^{\dagger}\right] = \delta_{kk'}$  and  $\left[a_{k}^{\dagger}, a_{k'}\right] = -\delta_{kk'}$ .

So, it is possible to find a common set of eigenstates for all of those commuting operators. These states are fully characterized by specifying the particle set of occupation number  $\{n_p\}$ , e.g.

$$\hat{n}_i |\{n_k\}\rangle = n_i |\{n_k\}\rangle$$
, (2.211)

and

$$N |\{n_k\}\rangle = \sum_l n_l |\{n_k\}\rangle$$
 (2.212)

So, the states  $|\{n_k\}\rangle$  form the basis of the Hilbert space. This description of a Hilbert space, in which the base vectors are chosen as eigenstates of number operators *N* and  $\hat{n}_k$ , is called a *Fock space* representation.  $\mathcal{H}$  may also be though of as a direct sum of subspaces  $\mathcal{H}_N$ , each made up of states with total occupation number  $N = \sum_k n_k$ :

$$\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1 \oplus \mathcal{H}_2 \oplus \ldots = \bigoplus_{N=0}^{\infty} \mathcal{H}_N.$$
 (2.213)

From its very definition the structure of  $|\{n_p\}\rangle$  is

$$|\{n_p\}\rangle = \prod_p (n_p!)^{-1/2} [a^{\dagger}(p)]^{n_p} |0\rangle$$
 (2.214)

Action of  $a_k^{\dagger} = a^{\dagger}(k)$  on  $|\{n_p\}\rangle$  can be expressed as

$$a_{k}^{\dagger} |\{n_{p}\}\rangle = \frac{a_{p_{1}}^{\dagger n_{p_{1}}}}{\sqrt{n_{p_{1}}!}} \dots \frac{a_{k}^{\dagger n_{k}+1}}{\sqrt{n_{k}!}} \dots |0\rangle$$
$$= \frac{\sqrt{(n_{k}+1)!}}{\sqrt{n_{k}!}} \left[ \frac{a_{p_{1}}^{\dagger n_{p_{1}}}}{\sqrt{n_{p_{1}}!}} \dots \frac{a_{k}^{\dagger n_{k}+1}}{\sqrt{n_{k}+1!}} \dots |0\rangle \right]$$
$$= \sqrt{n_{k}+1} |n_{p_{1}}, n_{p_{2}}, \dots, n_{k}+1, \dots\rangle .$$
(2.215)

Similarly, action of the operator  $a_k$  on  $|\{n_p\}\rangle$  can be computed as follows

$$a_{k} |\{n_{p}\}\rangle = \sum_{\{n'\}} |\{n'\}\rangle \langle\{n'\}| a_{k} |\{n_{p}\}\rangle$$

$$= \sum_{\{n'\}} |\{n'\}\rangle \langle n_{p_{1}}, \dots | a_{k}^{\dagger} | n'_{p_{1}}, \dots \rangle^{*}$$

$$= \sum_{\{n'\}} \sqrt{n'_{k} + 1} \delta^{\hat{k}}_{\{n\}, \{n'\}} \delta_{n_{k}, n'_{k} + 1} |\{n'\}\rangle$$

$$= \sqrt{n_{k}} |n_{p_{1}}, \dots, n_{k} - 1, \dots\rangle . \qquad (2.216)$$

Symbol  $\delta_{\{n\},\{n'\}}^{\hat{k}}$  denotes the multi-Kronecker  $\delta$  between sets  $\{n\}$  and  $\{n'\}$  excluding element  $n_k$  for which a separate rule must be stated. In deriving (2.216) we have used the *resolution of unity* 

$$1 = \sum_{\{n\}} |\{n\}\rangle \langle \{n\}|$$
  
=  $|0\rangle \langle 0| + \sum_{\sum n_i = 1} |\{n\}\rangle \langle \{n\}| + \sum_{\sum n_i = 2} |\{n\}\rangle \langle \{n\}| \dots$  (2.217)

The resolution of unity can also be equivalently written in the form

$$1 = |0\rangle \langle 0| + \sum_{n=1}^{\infty} \frac{1}{n!} \prod_{i=1}^{n} \int \frac{d^{3} \boldsymbol{p}_{i}}{(2\pi)^{3} 2\omega_{\boldsymbol{p}_{i}}} |p_{1}, p_{2}, \dots, p_{n}\rangle \langle p_{1}, p_{2}, \dots, p_{n}| . \quad (2.218)$$

With this any state  $|\psi\rangle$  in the Fock space can be written as

$$|\psi\rangle = |0\rangle \langle 0|\psi\rangle + \sum_{n=1}^{\infty} \frac{1}{n!} \prod_{i=1}^{n} \int \frac{\mathrm{d}^{3} \boldsymbol{p}_{i}}{(2\pi)^{3} 2\omega_{\boldsymbol{p}_{i}}} f_{\psi}^{(n)}(p_{1}, \dots, p_{n}) |p_{1}, \dots, p_{n}\rangle , \quad (2.219)$$

Here  $f_{\psi}^{(n)}(p_1, \ldots, p_n)$  are *n*-point wave functions that are (as can be easily checked) symmetric in all their arguments. Note that  $|0\rangle$  is a vacuum state, i.e., state without any particle. The later is different from the vacuum in the 1st quantized theory (despite of a similar notation), which is the lowest-energy single-particle state. In particular, for the matrix element  $\langle 0 | \phi | \psi \rangle$  of the field operator we have

$$\begin{aligned} \langle 0 | \phi | \psi \rangle &= \langle 0 | \phi^{+}(x) | \psi \rangle \\ &= \langle 0 | \int \frac{\mathrm{d}^{3} \mathbf{k}}{(2\pi)^{3} 2\omega_{\mathbf{k}}} e^{-ikx} a(k) \int \frac{\mathrm{d}^{3} \mathbf{p}}{(2\pi)^{3} 2\omega_{\mathbf{p}}} | p \rangle f_{\psi}^{(1)}(p) \\ &= \int \frac{\mathrm{d}^{3} \mathbf{k} \mathrm{d}^{3} \mathbf{p}}{(2\pi)^{6} 2\omega_{\mathbf{k}} 2\omega_{\mathbf{p}}} e^{-ikx} f_{\psi}^{(1)}(p) 2\omega_{\mathbf{k}} (2\pi)^{3} \delta(\mathbf{k} - \mathbf{p}) \\ &= \int \frac{\mathrm{d}^{3} \mathbf{k}}{(2\pi)^{3} 2\omega_{\mathbf{k}}} e^{-ikx} f_{\psi}^{(1)}(k) \\ &= \int \frac{\mathrm{d}^{4} k}{(2\pi)^{4}} e^{-ikx} \delta(\mathbf{k} - \mathbf{p}) \theta(k_{0}) f_{\psi}^{(1)}(k) \\ &= \psi^{(1)}(x) . \end{aligned}$$
(2.220)

So,  $\psi^{(1)}(x)$  is a Fourier transform of the single-particle wave function (in momentum representation), which is nothing but a single-particle wave function from 1st quantization. On the other hand, the Klein–Gordon field satisfies the equation  $(\partial^2 + m^2)\hat{\phi} = 0$ , so we also have

$$\langle 0| \left(\partial^2 + m^2\right) \hat{\phi} |\psi\rangle = 0, \qquad (2.221)$$

which implies that  $(\partial^2 + m^2) \langle 0 | \hat{\phi} | \psi \rangle = (\partial^2 + m^2) \psi^{(1)} = 0$ . This,  $\psi^{(1)}$  correctly satisfies the Klein–Gordon equation, as the scalar-particle

In (2.218)  $p_i$ 's are not organized in descendent order. To prove the relation use the fact that:

$$\langle p_1, \dots, p_n | q_1, \dots, q_n \rangle$$
  
=  $\sum_{\pi(j)} \prod_i (2\pi)^3 2\omega_{\mathbf{p}\,i} \,\delta(\mathbf{p}_i - \mathbf{q}_{\pi(j)})$ 

and act with (2.218) on arbitrary energy eigenstate, and observe that the same state is retrieved.

Note that  $\langle \psi | \hat{\phi} | 0 \rangle$  also satisfies Klein– Gordon equation but in this case it corresponds to negative-energy singleparticle wave function. wave function should. This provides a very important lesson. Free field itself must satisfy the 1st quantized wave equation because its single-particle matrix element satisfies it. This will give us a useful guide for selecting logically consistent field theories.

In passing we note one terminological issue. The fact that free fields satisfy the same equations as corresponding single-particle wave functions has been reason why QFT is sometimes called *second quantization*. While in *first quantization* we quantize classical single (or a few)-particle atributes:  $x, p, \ldots \rightarrow \hat{x}, \hat{p}, \ldots$ , in the second quantization we formally "quantize" the wave function:  $\psi \rightarrow \hat{\phi}$ .

# 2.8 Quantization of the Dirac Field

Dirac field describes Fermions with spin  $\frac{1}{2}$  (e.g., electron or positron), which (as will be seen shortly) posses antisymmetric statistics (justifying, in turn, the spin-statistics theorem). In order to quantize this field, we can start with a classical field Lagrangian. Since we know that the field must satisfy the 1st quantized wave equation (so as to yield the correct one-particle state equation) we should use the Lagrangian that can reproduce Dirac's equation. The later has the form

$$L = \int d^3 \mathbf{x} \underbrace{\overline{\psi}(x)}_{\psi^{\dagger}(x)\gamma^0} \left( i\gamma^{\mu}\partial_{\mu} - m \right) \psi(x) \,. \tag{2.222}$$

In analogy with the complex scalar field we treat  $\psi(x)$  and  $\overline{\psi}(x)$  as independent fields. Now, we wish to compute fields canonically conjugate to  $\psi(x)$  and  $\overline{\psi}(x)$ . Following the usual recipe, we get

$$\pi_{\alpha}(x) \equiv \chi_{\alpha}(x) = \frac{\delta L}{\delta \dot{\psi_{\alpha}}(x)} = \left(i\overline{\psi}(x)\gamma^{0}\right)_{\alpha} = i\overline{\psi}_{\beta}(x)\gamma^{0}_{\beta\alpha} = i\psi^{\dagger}(x)_{\alpha}.$$
 (2.223)

Note, that  $\overline{\psi}(x)$  does not appear in the Lagrangian (!) and so there is no field conjugated to  $\overline{\psi}(x)$ , i.e.  $\overline{\chi} = 0$ . At this stage one may expect, that the commutation rule is of the form

$$\left[\psi_{\alpha}(\boldsymbol{x},t),\chi_{\beta}(\boldsymbol{y},t)\right] = i\delta(\boldsymbol{x}-\boldsymbol{y})\delta_{\alpha\beta}, \qquad (2.224)$$

or equivalently

$$\left[\psi_{\alpha}(\boldsymbol{x},t),\psi_{\beta}^{\dagger}(\boldsymbol{y},t)\right] = \delta_{\alpha\beta}\delta(\boldsymbol{x}-\boldsymbol{y}).$$
(2.225)

We shall, however, see shortly that one has to use anticommutators in the Dirac theory.

The Hamiltonian is given by

$$H = \int d^{3}x (\chi \dot{\psi} + \underbrace{\chi \dot{\psi}}_{=0}) - L$$
  
= 
$$\int d^{3}x \left( i\overline{\psi}\gamma^{0}\dot{\psi} - \overline{\psi}i\gamma^{\mu}\partial_{\mu}\psi + m\overline{\psi}\psi \right)$$
  
= 
$$\int d^{3}x \left( i\overline{\psi}\gamma\nabla\psi + m\overline{\psi}\psi \right)$$
  
= 
$$\int d^{3}x \psi^{\dagger} \left( i\gamma^{0}\gamma\nabla + m\gamma^{0} \right)\psi. \qquad (2.226)$$

Here  $\gamma = (\gamma^1, \gamma^2, \gamma^3)$ . By employing the properties of  $\gamma$ -matrices and integrating per-partes we see from the last identity that the Hamiltonin is clearly Hermitian (as it should). With the Hamiltonian we can write in the Heisenberg-picture the standard Heisenberg equations of motion

$$\dot{\psi} = i \left[ H, \psi \right] = i \int d^3 x \left[ i \overline{\psi} \gamma \nabla \psi + m \overline{\psi} \psi, \psi \right] .$$
(2.227)

Now, because the fields satisfy the Dirac (and hence the Klein–Gordon) equation, the solution can be written in the form

$$\psi(x) = \sum_{p} \left( A(p)e^{-ipx} + B(p)e^{ipx} \right)$$
  
$$= \sum_{p} \left( \sum_{\lambda \in \{1,2\}} a(p,\lambda)u(p,\lambda)e^{-ipx} + \sum_{\lambda \in \{1,2\}} b^{*}(p,\lambda)v(p,\lambda)e^{ipx} \right)$$
  
$$= \sum_{p} \sum_{\lambda} \left( a(p,\lambda)u(p,\lambda)e^{-ipx} + b^{*}(p,\lambda)v(p,\lambda)e^{ipx} \right). \quad (2.228)$$

Here,  $\lambda$  is the helicity index. Eq. (2.228) immediately implies that

$$\overline{\psi}(x) = \psi^{\dagger}(x)\gamma^{0}$$
$$= \sum_{p} \sum_{\lambda} \left( b(p,\lambda)\overline{\nu}(p,\lambda)e^{-ipx} + a^{*}(p,\lambda)\overline{u}(p,\lambda)e^{ipx} \right). \quad (2.229)$$

Let us recall that we have already derived the following orthogonality relations:

$$\begin{split} \overline{u}(p,\lambda)u(p,\lambda') &= 2m\delta_{\lambda\lambda'}, \\ \overline{v}(p,\lambda)v(p,\lambda') &= -2m\delta_{\lambda\lambda'}, \\ \overline{u}(p,\lambda)v(p,\lambda') &= 0, \\ \overline{v}(p,\lambda)u(p,\lambda') &= 0, \\ \overline{u}(p,\lambda)\gamma^{0}u(p,\lambda') &= 2\omega_{p}\delta_{\lambda\lambda'}, \\ \overline{v}(p,\lambda)\gamma^{0}v(p,\lambda') &= 2\omega_{p}\delta_{\lambda\lambda'} \text{ (No change of sign!).} \quad (2.230) \end{split}$$

To quantize, we promote  $\psi(x)$  and  $\overline{\psi}(x)$  to operators (along with  $a, a^*$  and  $b, b^*$ , which are promoted to the  $a, a^{\dagger}$  and  $b, b^{\dagger}$ ). This also promotes Hamiltonian to the operator. The above mode expansion of  $\psi$  and  $\overline{\psi}$ 

Recall that  $(p - m)u(p, \lambda) = 0$  and  $(p + m)v(p, \lambda) = 0$ .

allows to formulate *H* entirely in the language of a,  $a^{\dagger}$  and b,  $b^{\dagger}$ . Consequently, *H* can be rewritten in terms of "creation" and "annihilation" operators as

$$H = \sum_{\boldsymbol{p},\lambda} \omega_p \left( a_{\lambda}^{\dagger}(p) a_{\lambda}(p) - b_{\lambda}(p) b_{\lambda}^{\dagger}(p) \right) .$$
 (2.231)

Should we now used the presumed *commutation* rules for  $\psi$  and  $\overline{\psi}$ , then it can be easily checked that  $a, a^{\dagger}$  and  $b, b^{\dagger}$  would obey the commutation rules as well. This leads, however, to the problem since the ensuing Hamiltonian would not be positive (even worse, it would be unbounded from below). The particles a and b contribute opposite sign to the energy, which means that this theory would not admit a stable ground state. If we however assume that anticommutation relations hold:

$$\left\{ a_{\lambda}(p), a_{\lambda'}^{\dagger}(p') \right\} = \delta_{\lambda\lambda'} \delta_{pp'},$$

$$\left\{ b_{\lambda}(p), b_{\lambda'}^{\dagger}(p') \right\} = \delta_{\lambda\lambda'} \delta_{pp'},$$

$$\left\{ a_{\lambda}^{\dagger}(p), a_{\lambda'}^{\dagger}(p') \right\} = \left\{ a_{\lambda}(p), b_{\lambda'}(p') \right\} = \dots = 0,$$

$$(2.232)$$

the Hamiltonian can be written as

$$H = \sum_{\boldsymbol{p},\lambda} \omega_p \left( a_{\lambda}^{\dagger}(\boldsymbol{p}) a_{\lambda}(\boldsymbol{p}) + b_{\lambda}^{\dagger}(\boldsymbol{p}) b_{\lambda}(\boldsymbol{p}) \right) - \sum_{\boldsymbol{p}} 2 \omega_p \delta_{\boldsymbol{p} \boldsymbol{p}'} \,. \tag{2.233}$$

Now, it seems that we needed only anticommutation rule for *b* particles, but because  $\psi(x)$  and  $\overline{\psi}(x)$  involve the sum over *a* and  $b^{\dagger}$  as well as  $a^{\dagger}$  and *b*, we must take *a* and  $a^{\dagger}$  to have anticommutation rules as well in order to have anticommutation rule  $\psi(x)$  and  $\overline{\psi}(x)$ . The later is, in turn, consistent with various physical requirements (e.g., only with anticommutations rule we get correct Dirac's equation of motion for Heisenberg fields  $\psi(x)$  and  $\overline{\psi}(x)$ ). It can be checked, that with the rules (2.232) the following anticommutation relations hold for the canonically conjugate fields

$$\{\psi_{\alpha}(\boldsymbol{x},t),\chi_{\beta}(\boldsymbol{y},t)\} = i\delta_{\alpha\beta}\delta(\boldsymbol{x}-\boldsymbol{y}),$$
  
$$\Leftrightarrow \qquad \{\psi_{\beta}^{\dagger}(\boldsymbol{x},t),\psi_{\alpha}(\boldsymbol{y},t)\} = \delta_{\alpha\beta}\delta(\boldsymbol{x}-\boldsymbol{y}), \qquad (2.234)$$

and also

$$\{\psi,\psi\} = \{\psi^{\dagger},\psi^{\dagger}\} = 0.$$
 (2.235)

In passing we might notice that (2.234) implies

$$\left\{\psi_{\alpha}(\boldsymbol{x},t),\overline{\psi}_{\beta}(\boldsymbol{y},t)\right\} = \gamma^{0}_{\alpha\beta}\delta(\boldsymbol{x}-\boldsymbol{y}).$$
(2.236)

Let us now see that these anticommutation rules provide expected equation of motion — Dirac's equation. To this end we need to compute the Heisenberg equations of motion for fields, i.e.

$$\dot{\psi} = i [H, \psi] = i \int d^3 \mathbf{x}' \left[ i \overline{\psi} \gamma \nabla \psi + m \overline{\psi} \psi, \psi \right].$$
(2.237)

First, let us calculate (equal time is implicitly assumed)

$$\begin{split} \left[\overline{\psi}(x')\psi(x'),\psi_{\beta}(x)\right] &= \overline{\psi}_{\alpha}(x')\{\psi_{\alpha}(x'),\psi_{\beta}(x)\} - \{\overline{\psi}_{\alpha}(x'),\psi_{\beta}(x)\}\psi_{\alpha}(x')\\ &= -\delta(\mathbf{x}'-\mathbf{x})\gamma_{\beta\alpha}^{0}\psi_{\alpha}(x')\,. \end{split}$$
(2.238)

Here we have used the identity  $[AB, C] = A\{B, C\} - \{A, C\}B$ . The second commutator we need is

$$\begin{bmatrix} i\overline{\psi}_{\alpha}(x')\gamma_{\alpha\delta}\nabla'\psi_{\delta}(x'),\psi_{\beta}(x) \end{bmatrix} = -i\{\overline{\psi}_{\alpha}(x'),\psi_{\beta}(x)\}\gamma_{\alpha\delta}\nabla'\psi_{\delta}(x') \\ = -i\delta(\mathbf{x}'-\mathbf{x})\gamma_{\beta\alpha}^{0}\gamma_{\alpha\delta}\nabla'\psi_{\delta}(x'). \quad (2.239)$$

This togehter leads to

$$\begin{split} \dot{\psi}_{\beta} &= i \int d^{3}\boldsymbol{x}' \left[ i \overline{\psi} \boldsymbol{\gamma} \nabla \psi + m \overline{\psi} \psi, \psi \right] \\ &= i \int d^{3}\boldsymbol{x}' \left\{ i (-(\gamma^{0} \boldsymbol{\gamma})_{\beta \delta} \nabla' \psi_{\delta}(\boldsymbol{x}')) - m \gamma^{0}_{\beta \alpha} \psi_{\alpha}(\boldsymbol{x}') \right\} \delta(\boldsymbol{x}' - \boldsymbol{x}) \\ &= i \left[ -i (\gamma^{0} \boldsymbol{\gamma} \nabla \psi(\boldsymbol{x}))_{\beta} - m (\gamma^{0} \psi(\boldsymbol{x}))_{\beta} \right] \\ &= \left[ \gamma^{0} \boldsymbol{\gamma} \nabla \psi(\boldsymbol{x}) - i m \gamma^{0} \psi(\boldsymbol{x}) \right]_{\beta} , \end{split}$$
(2.240)

which is the Heisenberg equation of motion. Multiplying this by  $i\gamma^0$  we get

$$i\gamma^{0}\dot{\psi}(x) = i\gamma\nabla\psi(x) + m\psi(x)$$
  

$$\Leftrightarrow \quad i(\gamma^{0}\partial_{0}\psi(x) - \gamma\nabla\psi(x)) - m\psi(x) = 0$$
  

$$\Leftrightarrow \quad (i\gamma^{\mu}\partial_{\mu} - m)\psi(x) = 0. \quad (2.241)$$

Hence, the Heisenberg equation of motion correctly produces Dirac's equation.

## **Energy-momentum tensor**

Note that when Dirac's field obeys the equation of motion, the Lagrangian vanishes (L = 0). In such a case we write the formula for the Hamiltonian in the form

$$H = \int d^3 \mathbf{x} \, i \overline{\psi}(x) \gamma^0 \dot{\psi}(x) \,. \tag{2.242}$$

At this point we can introduce the tensor

$$T^{\mu\nu} = i\overline{\psi}(x)\gamma^{\mu}\partial^{\nu}\psi(x), \qquad (2.243)$$

(which is not symmetric in  $\mu \nu$ !). Note that  $T^{\mu\nu}$  satisfies on-shell the continuity equation

$$\partial_{\mu}T^{\mu\nu} = i\left(\partial_{\mu}\overline{\psi}(x)\gamma^{\mu}\right)\partial^{\nu}\psi(x) + i\overline{\psi}(x)\partial^{\nu}\left(\partial_{\mu}\gamma^{\mu}\psi(x)\right)$$
$$= -im\overline{\psi}(x)\psi(x) + im\overline{\psi}(x)\psi(x) = 0.$$
(2.244)

This allows us to define the 4-vector  $P^{\nu}$  as

$$P^{\nu} = \int d^3 x T^{0\nu}(x), \qquad (2.245)$$

which for the space-like components (i.e., 3-momentum) reads as

$$\boldsymbol{P} = -i \int d^3 \boldsymbol{x} \overline{\psi}(x) \gamma^0 \nabla \psi(x)$$
  

$$\Leftrightarrow \qquad \boldsymbol{P}^i = i \int d^3 \boldsymbol{x} \psi^{\dagger}(x) \partial^i \psi(x). \qquad (2.246)$$

It can be checked that  $P^{\mu}$  satisfies the correct relation

$$e^{iPa}\psi(x')e^{-iPa} = \psi(x+a), \qquad (2.247)$$

(and similarly for  $\overline{\psi}$ ) which in turn implies that  $P^{\mu}$  must be a generator of space-time translations, or in other words, it is the *total 4-momentum*.

Relation (2.247) can be proved most easily by looking at the ensuing infinitesimal version. Namely, for  $|a^{\mu}| \ll 1$  we have to the linear order in  $a^{\mu}$ 

$$\partial_{\mu}\psi(x) = i \left[ P_{\mu}, \psi(x) \right] ,$$
  
$$\partial_{\mu}\overline{\psi}(x) = i \left[ P_{\mu}, \overline{\psi}(x) \right] . \qquad (2.248)$$

A direct computation reveals that (2.246) indeed satisfies both relations (2.248). Note that the 0th component of (2.248) is nothing but the Heisenberg equation of motion.

Properties (2.244), (2.245) and (2.247) allow to identify  $T^{\mu\nu}$  with energymomentum tensor. A constructive way towards construction of  $T^{\mu\nu}$ will be discussed in connection with Noether's theorem.

In passing we note that from 1st quantization we know that there exists a conserved current. By replacing the wave function with quantum field we have

$$J_{\mu}(x) = \overline{\psi} \gamma_{\mu} \psi(x). \qquad (2.249)$$

Again as in 1st quantization, by using the equation of the motion one can show that

$$\partial_{\mu}J^{\mu}(x) = 0,$$
 (2.250)

and that

$$Q \equiv \int \mathrm{d}^3 \boldsymbol{x} J^0(\boldsymbol{x}, t) \,, \qquad (2.251)$$

is such that

$$[H,Q] = 0. (2.252)$$

i.e., Q is conserved charge. Note that in the 1st quantization Q represented total probability while now Q is an operator. The actual meaning of Q will become clear in the following section.

#### 4-Momentum and charge *Q* — further discussion

Let us now rephrase  $P^{\nu}$  in terms of creation and annihilation operators. We find (not too surprisingly) that

$$P^{\nu} = \sum_{\boldsymbol{p},\lambda} p^{\nu} \left[ a^{\dagger}_{\lambda}(\boldsymbol{p}) a_{\lambda}(\boldsymbol{p}) - b_{\lambda}(\boldsymbol{p}) b^{\dagger}_{\lambda}(\boldsymbol{p}) \right].$$
(2.253)

With this we can easily check that

$$P^{\nu}a^{\dagger}_{\lambda}(p) = [P^{\nu}, a^{\dagger}_{\lambda}(p)] + a^{\dagger}_{\lambda}(p)P^{\nu}$$
$$= a^{\dagger}_{\lambda}(p)(P^{\nu} + p^{\nu}). \qquad (2.254)$$

And similarly for  $P^{\nu}b_{\lambda}^{\dagger}(p) = b_{\lambda}^{\dagger}(p)(P^{\nu} + p^{\nu})$ . Hence,  $a_{\lambda}^{\dagger}(p)$  and  $b_{\lambda}^{\dagger}(p)$  create particles with the corresponding momentum and helicity.

Similarly, we also get

$$P^{\nu}a_{\lambda}(p) = a_{\lambda}(p)(P^{\nu} - p^{\nu}),$$
  

$$P^{\nu}b_{\lambda}(p) = b_{\lambda}(p)(P^{\nu} - p^{\nu}).$$
(2.255)

Thus,  $a_{\lambda}(p)$  and  $b_{\lambda}(p)$  annihilate particles with the corresponding momentum and helicity.

Again, we wish  $|0\rangle$  to have zero energy and momenta, i.e.  $P^{\nu} |0\rangle = 0$ . This can be done via *normal ordering* (which subtracts vacuum energy):

$$P^{\nu} = \int d^3 x T^{0\nu}, \quad \text{where} \quad T^{\mu\nu} = i : \overline{\psi}(x) \gamma^{\mu} \partial^{\nu} \psi(x) : . \quad (2.256)$$

In the context of Dirac fields, normal ordering requires that we place annihilation operator to the right and creation operators to the left, but insert a factor of -1 for each operator interchange, e.g.

$$P^{\nu} = : \sum_{p,\lambda} p^{\nu} \{ a^{\dagger}_{\lambda}(p) a_{\lambda}(p) - b_{\lambda}(p) b^{\dagger}_{\lambda}(p) \} :$$
$$= \sum_{p,\lambda} p^{\nu} \{ a^{\dagger}_{\lambda}(p) a_{\lambda}(p) + b^{\dagger}_{\lambda}(p) b_{\lambda}(p) \} .$$
(2.257)

This should be compared with non-normally ordered  $P^{\nu}$ 

$$P^{\nu} = \sum_{p,\lambda} p^{\nu} [a^{\dagger}_{\lambda}(p)a_{\lambda}(p) + b^{\dagger}_{\lambda}(p)b_{\lambda}(p) - \delta_{pp}\delta_{\lambda\lambda}]. \qquad (2.258)$$

By noting that

$$-\sum_{\boldsymbol{p},\lambda} p^{\nu} \delta_{\boldsymbol{p}\boldsymbol{p}} \delta_{\lambda\lambda} = -2 \int \frac{\mathrm{d}^{3}\boldsymbol{p}}{(2\pi)^{3} 2\omega_{\boldsymbol{p}}} p^{\nu} (2\pi)^{3} 2\omega_{\boldsymbol{p}} V$$
$$= -2 \int \mathrm{d}^{3}\boldsymbol{p} p^{\nu} V = \langle 0|P^{\nu}|0\rangle . \qquad (2.259)$$

we see that again

$$P^{\nu} \rightarrow : P^{\nu} := P^{\nu} - \langle 0 | P^{\nu} | 0 \rangle . \qquad (2.260)$$

For spatial components  $\langle 0|\mathbf{P}|0\rangle = 0$ , and so we need the normal ordering only for  $P^0 = H$ .

Strictly speaking, the normal ordering should be now employed for any composite operator. In particular, we should also normally order the conserved charge Q (cf. Eq. (2.251)). So, we should write

$$Q = : \int d^3 x J^0(x) := : \int d^3 x \psi^{\dagger}(x) \psi(x) : .$$
 (2.261)

We can again show that

$$Q = \sum_{\boldsymbol{p},\lambda} \left[ a_{\lambda}^{\dagger}(\boldsymbol{p}) a_{\lambda}(\boldsymbol{p}) - b_{\lambda}^{\dagger}(\boldsymbol{p}) b_{\lambda}(\boldsymbol{p}) \right].$$
(2.262)

With this we obtain

$$Qa^{\dagger}_{\lambda}(p) = a^{\dagger}_{\lambda}(p)Q + \left[Q, a^{\dagger}_{\lambda}(p)\right] = a^{\dagger}_{\lambda}(p)(Q+1),$$
  

$$Qb^{\dagger}_{\lambda}(p) = b^{\dagger}_{\lambda}(p)Q + \left[Q, b^{\dagger}_{\lambda}(p)\right] = b^{\dagger}_{\lambda}(p)(Q-1). \quad (2.263)$$

Let us remind that  $a^{\dagger}_{\lambda}(p)$  and  $b^{\dagger}_{\lambda}(p)$  create particles of type *a* and *b* with the equal 4-momenta (hence also equal rest mass) and helicity. In this respect particles *a* and *b* are identical. Now from (2.263) we see that they are not entirely identical because  $a^{\dagger}_{\lambda}(p)$  and  $b^{\dagger}_{\lambda}(p)$  create particles with opposite charge. It will be seen that *Q* can be identified with the electric charge. Consequently *a* and *b* are antiparticles to each other. Conventionally we will call particles of the type *a* as *particles* and particles of type *b* as *antiparticles*.

#### **Spin-statistics connection**

Due to the canonical relations  $\{a_p^{\dagger}, a_q^{\dagger}\} = \{a_p, a_q\} = \{b_p^{\dagger}, b_q^{\dagger}\} = \{b_p, b_q\} = 0$  we see that only possible occupation number of a state  $|\cdots p, \lambda \cdots \rangle$  is 0 or 1. Indeed, take

$$|p_1, \lambda_1, p_2, \lambda_2 \cdots, p, \lambda \cdots \rangle = |\cdots \underbrace{0}_{p, \lambda} \cdots \rangle.$$

Now by action with creation operator

$$a_{\lambda}^{\dagger}(p) | \cdots 0 \cdots \rangle = C | \cdots \underbrace{1}_{p,\lambda} \cdots \rangle ,$$

but

$$\cdots \underbrace{2}_{p,\lambda} \cdots \rangle = \frac{1}{\sqrt{2}} \underbrace{a_{\lambda}^{\dagger}(p) a_{\lambda}^{\dagger}(p)}_{=0} | \cdots \underbrace{0}_{p,\lambda} \cdots \rangle.$$

Thus, we cannot create a state with the occupation number  $n_p \ge 2$ . Similarly for particle with an opposite-charge state (antiparticle state) generated  $b^{\dagger}_{\lambda}(p)$ .

Field theory of Dirac fields (spin  $\frac{1}{2}$ ) automatically prescribes (or implies) Pauli's exclusion principle, i.e. Dirac fields need to obey Fermi–Dirac statistics.

# 2.9 Symmetry and Conserved Currents, Noether's Theorem

In field theory (both classical and quantum), symmetries and conservation laws are related. Our starting point is Lagrangian

$$L = \int d^3 \mathbf{x} \mathcal{L}(\phi_r(x), \partial_\mu \phi_r(x)), \qquad (2.264)$$

with the ensuing equation of motion

$$\partial_{\mu} \left( \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi_r)} \right) - \frac{\partial \mathcal{L}}{\partial \phi_r} = 0.$$
 (2.265)

Any continuous symmetry transformation, which leaves the Lagrangian  $\mathcal{L}$  invariant implies the existence of a current satisfying equation of continuity

$$\partial_{\mu}J^{\mu}(x) = 0, \qquad (2.266)$$

This in turn defines the charge

$$Q = \int d^3 x J^0(x, t), \qquad (2.267)$$

that is conserved, because the surface term at infinity is negligibly small, i.e.

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = \int \mathrm{d}^3 \boldsymbol{x} \partial_0 J^0 = \int \mathrm{d}^3 \boldsymbol{x} \boldsymbol{\nabla} \cdot \boldsymbol{J} = 0. \qquad (2.268)$$

Particularly important is the case when the Lagrangian is invariant with respect to internal symmetry, i.e., symmetry transformation that acts on the internal indices r. In other words, the action is invariant under transformation

$$\phi_r(x) \to \phi'_r(x) = \phi_r(x) + \delta \phi_r(x). \qquad (2.269)$$

Let us recall that for Lorentz group we had

$$\psi(x) \xrightarrow{L} \psi'(x) = S(L)\psi(L^{-1}x) = S_{\alpha\beta}(L)\psi_{\beta}(L^{-1}x)$$
$$= \left(e^{i\omega_{\mu\nu}M^{\mu\nu}}\right)_{\alpha\beta}\psi_{\beta}(L^{-1}x).$$
(2.270)
Similarly, under the group of internal symmetries  $\phi_r(x) \xrightarrow{G} \phi'_r(x)$ :

$$\phi_{r}(x) \xrightarrow{\mathbf{G}} \phi_{r}'(x) = S(\mathbf{G})_{rq} \phi_{q}(x) = \left(e^{i\epsilon^{a} \mathbf{T}^{a}}\right)_{rq} \phi_{q}(x)$$

$$\stackrel{|\epsilon|\ll 1}{=} (\mathbf{1} + i\epsilon^{a} \mathbf{T}^{a})_{rq} \phi_{q}(x)$$

$$= \phi_{r}(x) + \underbrace{i\epsilon^{a} \mathbf{T}^{a}_{rq} \phi_{q}(x)}_{\delta\phi_{r}(x)}, \qquad (2.271)$$

where  $\epsilon^a$  are (*x*-independent) small parameters and  $T^a$  are generators of the Lie group *G* satisfying

$$\left[\boldsymbol{T}^{a}, \boldsymbol{T}^{b}\right] = ic^{abc}\boldsymbol{T}^{c} . \qquad (2.272)$$

Here  $c^{abc}$  are the so-called *structure constants* of *G*. If the Lagrangian is unchanged under the action of the group *G*, then  $\delta \mathcal{L} = 0$  also for infinitesimal changes  $\delta \phi_r(x)$  specified above, i.e.

$$0 = \delta \mathcal{L}(x) = \int dy \frac{\delta \mathcal{L}(x)}{\delta \phi_r(y)} \delta \phi_r(y). \qquad (2.273)$$

Functional derivative can be explicitly written as

$$\frac{\delta \mathcal{L}(x)}{\delta \phi_r(y)} = \frac{\mathrm{d}}{\mathrm{d}\epsilon_r} \mathcal{L}_x(\phi_r + \epsilon_r \delta(x - y), \partial_\mu \phi_r + \partial_\mu \epsilon_r \delta(x - y)) \bigg|_{\epsilon_r = 0}$$
$$= \frac{\partial \mathcal{L}(x)}{\partial \phi_r(x)} \delta(x - y) + \frac{\partial \mathcal{L}(x)}{\partial (\partial_\mu \phi_r(x))} \partial_\mu \delta(x - y).$$
(2.274)

So, when we employ the equations of motion we obtain

$$0 = \delta \mathcal{L} = \partial_{\mu} \left[ \frac{\partial \mathcal{L}}{\partial(\partial_{\mu}\phi_{r}(x))} \right] \delta\phi_{r}(x) + \frac{\partial \mathcal{L}}{\partial(\partial_{\mu}\phi_{r}(x))} \partial_{\mu}\delta\phi_{r}(x)$$
$$= \partial_{\mu} \left[ \frac{\partial \mathcal{L}}{\partial(\partial_{\mu}\phi_{r}(x))} \delta\phi_{r}(x) \right]$$
$$= \epsilon^{a} \partial_{\mu} \left[ \frac{\partial \mathcal{L}}{\partial(\partial_{\mu}\phi_{r}(x))} i T^{a}_{rq} \phi_{q}(x) \right]. \qquad (2.275)$$

Since this is true for arbitrary  $\epsilon^a$  we can identify a conserved 4-vector quantity (conserved current) satisfying continuity equation  $\partial_{\mu}J^{\mu}(x) = 0$ . So, one can identify a conserved current  $J^{\mu}$  as

$$J^{a}_{\mu}(x) = -i \frac{\partial \mathcal{L}}{\partial (\partial^{\mu} \phi_{r})} T^{a}_{rq} \phi_{q}(x), \qquad (2.276)$$

where -i is a conventional multiplicative factor. The conserved charges are thus given by

$$Q^{a} = \int d^{3}x J_{0}^{a}(x) , \qquad (2.277)$$

and are (apart from being conserved —  $\dot{Q}^a = 0$ ) also generators of the symmetry group. Currents  $J^a_{\mu}(x)$  and charges  $Q^a$  are known as *Noether currents* and *charges*, respectively.

Let us further note that

$$J^{a0} = -i\pi_r T^a_{rq} \phi_q \,. \tag{2.278}$$

From the canonical commutation relation

$$[\phi_a(\mathbf{x},t),\pi_b(\mathbf{y},t)] = i\delta_{ab}\delta(\mathbf{x}-\mathbf{y}).$$
(2.279)

it can be then deduced that

 $\left[J^{a0}(\mathbf{x},t), J^{b0}(\mathbf{y},t)\right] = ic^{abc} J^{c0}(\mathbf{x},t) \delta(\mathbf{x}-\mathbf{y}).$ (2.280)

By integrating this realation twice on LHS and RHS we obtain

$$\int d^{3}x d^{3}y \left[ J^{a0}(x,t), J^{b0}(y,t) \right] = ic^{abc} \int d^{3}x d^{3}y J^{c0}(x) \delta(x-y)$$
$$= ic^{abc} Q^{c} . \qquad (2.281)$$

Which finally yields

$$\left[Q^a, Q^b\right] = ic^{abc}Q^c \,. \tag{2.282}$$

So, the charges satisfy the same algebra as the original generators  $T^a$  of the symmetry.

As an illustrative example we consider Lagrangian of the form

$$\mathcal{L} = \frac{1}{2} \left[ (\partial_{\mu} \phi_1)^2 + (\partial_{\mu} \phi_2)^2 \right] - \frac{1}{2} m^2 \left( \phi_1^2 + \phi_2^2 \right) - \frac{1}{4} \lambda \left( \phi_1^2 + \phi_2^2 \right)^2.$$
(2.283)

This is invariant under 2D-rotation transformation

$$\phi_1 \rightarrow \phi'_1 = \phi_1 \cos \alpha - \phi_2 \sin \alpha,$$
  

$$\phi_2 \rightarrow \phi'_2 = \phi_1 \sin \alpha + \phi_2 \cos \alpha,$$
(2.284)

which can be succinctly written as

$$\begin{pmatrix} \phi_1' \\ \phi_2' \end{pmatrix} = \begin{pmatrix} \cos \alpha & -\sin \alpha \\ \sin \alpha & \cos \alpha \end{pmatrix} \begin{pmatrix} \phi_1 \\ \phi_2 \end{pmatrix}.$$
 (2.285)

Here the rotation matrix is an element of  $SO(2) \sim U(1)$  group. In this case we can write

$$G(\alpha) = e^{-i\alpha T}, \qquad (2.286)$$

where the corresponding group generator can be extracted via the usual prescription

$$T = -i \left. \frac{\mathrm{d}G(\alpha)}{\mathrm{d}\alpha} \right|_{\alpha=0} = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}. \tag{2.287}$$

For  $|\alpha| \ll 1$  we get

$$\phi'_{r} = \phi_{r} + i\alpha T_{rq}\phi_{q} = (1 + i\alpha T)_{rq}\phi_{q}, \qquad (2.288)$$

These generators act on a different representation space than  $T^a$ ,  $T^b$  and  $T^c$ . While *T*'s act on *internal space*, *Q*'s act directly on the Hilbert space.

Eq. (2.280) is an example of a so-called

current algebra.

and hence in this case our conserved current acquires the form

$$J_{\mu} = -i \frac{\partial \mathcal{L}}{\partial (\partial^{\mu} \phi_{r})} T_{rq} \phi_{q} . \qquad (2.289)$$

Knowing that only  $T_{12} = -T_{21} \neq 0$  we can write

$$J_{\mu} = -i \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi_{1})} T_{12} \phi_{2} - i \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi_{2})} T_{21} \phi_{1}$$
$$= (\partial_{\mu} \phi_{1}) \phi_{2} - (\partial_{\mu} \phi_{2}) \phi_{1}. \qquad (2.290)$$

The previous analysis can be alternatively (and conveniently) formulated in terms of complex (or non-Hermitian) fields defined as

$$\phi = \frac{1}{\sqrt{2}} (\phi_1 + i\phi_2),$$
  

$$\phi^{\dagger} = \frac{1}{\sqrt{2}} (\phi_1 - i\phi_2).$$
(2.291)

In this case we can rewrite our original Lagrangian as

$$\mathcal{L} = \left(\partial_{\mu}\phi^{*}\right)\left(\partial^{\mu}\phi\right) - m^{2}(\phi^{*}\phi) - \lambda(\phi^{*}\phi)^{2}.$$
(2.292)

This is clearly invariant under phase transformation

$$\begin{split} \phi &\to \phi' = e^{i\alpha}\phi \,, \\ \phi^* &\to \phi^{*\prime} = e^{-i\alpha}\phi^* \,, \end{split} \tag{2.293}$$

which we can again rewrite as

$$\begin{pmatrix} \phi'\\ \phi^{*\prime} \end{pmatrix} = \begin{pmatrix} e^{i\alpha} & 0\\ 0 & e^{-i\alpha} \end{pmatrix} \begin{pmatrix} \phi\\ \phi^{*} \end{pmatrix}.$$
 (2.294)

The ensuing group generator is

$$T = -i \left. \frac{\mathrm{d}G(\alpha)}{\mathrm{d}\alpha} \right|_{\alpha=0} = \left( \begin{array}{cc} 1 & 0\\ 0 & -1 \end{array} \right). \tag{2.295}$$

With this, we finally arrive at the conserved Noether current:

$$J_{\mu} = -i \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi)} T_{11} \phi - i \frac{\partial \mathcal{L}}{\partial (\partial_{\mu} \phi^{*})} T_{22} \phi^{*}$$
$$= i \left[ (\partial_{\mu} \phi) \phi^{*} - (\partial_{\mu} \phi^{*}) \phi \right]. \qquad (2.296)$$

Compare this formula with (1.42), which we had for the Klein–Gordon particle. Interpretation is, however, very different. In the first-quantized version  $J_{\mu}$  was a probability current with  $J_0 = \rho$  representing probability density. In the present (field-theory) case  $J_{\mu}$  represents a conserved current with  $J_0$  being density of the conserved charge. The charge associated with the U(1) symmetry is an *electric charge* and hence there is no surprise that conserved charge Q might be negative, positive or zero (as opposed to total probability in the first-quantized theory that must be positive and normalisable to unity).

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Note also that  $\phi_1$  and  $\phi_2$  (or  $\phi$  and  $\phi^*$ ) are degenerate in mass, because of the required  $U(1) \sim SO(2)$  symmetry.