Theoretical physics notes

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General information

Written & oral exam.

As opposed to what was done in the physics curriculum, here there will be no grade truncation: we can grade a grade up to a 30 with the written exam only.

The suggested book is D'Auria & Trigiante [DT11]. For the second part it is also useful to have a look at Mandl & Shaw [MS10].

Live question time in Zoom at half past 11 on Mondays.

Things which will be taken for granted: four-vectors, Lorenz and Poincaré groups, basics of QM, basics of linear operators.

Contents

This course will deal with the basics of Relativistic Quantum Field Theory.

We will discuss the Lagrangian formalism for a Classical Field Theory. We will quantize these theories using canonical quantization, specifically for a scalar, a Dirac fermion, and a vector boson.

Then, we will introduce interactions in our Lagrangian: we will use the S-matrix expansion, and Feynman diagrams.

Chapter 1

Relativistic Quantum Field Theory

1.1 The nonrelativistic wave equation

We will review the derivation of the nonrelativistic Schrödinger equation. We find it starting from the correspondence principle: we start from the expression of the energy

$$E = \frac{p^2}{2m} + V(x)\,, \tag{1.1}$$

and substitute the energy with $E \to i\partial_t$, the momentum with $\vec{p} \to -i\vec{\nabla}_x$ and the position with the position operator $\vec{x}$, all acting on the wavefunction. With this we get

$$i\frac{\partial\psi}{\partial t}(\vec{x},t) = \left(\frac{-\nabla^2}{2m} + V(\vec{x})\right)\psi(\vec{x},t)\,. \tag{1.2}$$

We still need to assign a meaning to the wavefunction: this is given by the Bohr condition, which tells us that the probability density of finding the particle in a specific region is

$$\rho(\vec{x},t) = \left|\psi(\vec{x},t)\right|^2 \geq 0\,. \tag{1.3}$$

This probability density must be normalized as an initial condition:

$$\mathbb{P}(t_0) = \int_{\mathbb{R}^3} \mathrm{d}^3x\, \rho(\vec{x},t_0) = 1\,, \tag{1.4}$$

and we wish to show that it will also be normalized at later times:

$$\frac{\mathrm{d}\mathbb{P}}{\mathrm{d}t} = \int_{\mathbb{R}^3} \mathrm{d}^3x\, \frac{\partial}{\partial t}\left|\psi(\vec{x},t)\right|^2 \tag{1.5a}$$

$$= \int_{\mathbb{R}^3} \mathrm{d}^3x \left(\psi^*\frac{\partial\psi}{\partial t} + \frac{\partial\psi^*}{\partial t}\psi\right). \tag{1.5b}$$

Using the Schrödinger equation we can substitute in the expression for the derivative of the wavefunction:

$$\frac{\mathrm{d}\mathbb{P}}{\mathrm{d}t} = \int_{\mathbb{R}^3} \mathrm{d}^3x \left\{\psi^*\frac{1}{i}\left(-\frac{\nabla^2}{2m} + V\right)\psi - \frac{1}{i}\psi\left(-\frac{\nabla^2}{2m} + V\right)\psi^*\right\} \tag{1.6a}$$

$$= \frac{i}{2m} \int_{\mathbb{R}^3} \mathrm{d}^3x \left\{ \psi^* \nabla^2 \psi - 2m\psi^* V\psi - \psi \nabla^2 \psi^* + 2m\psi V \psi^* \right\}, \tag{1.6b}$$

and we use the fact that

$$\psi^* V \psi = \psi V \psi^* = \left(\psi^* V \psi\right)^*, \tag{1.7}$$

which is true since V is a symmetric operator: it has real eigenvalues. This allows us to simplify the terms which include V, and we find:

$$\frac{\mathrm{d}\mathbb{P}}{\mathrm{d}t} = \frac{i}{2m} \int_{\mathbb{R}^3} \mathrm{d}^3x \left\{ \psi^* \nabla^2 \psi - \psi \nabla^2 \psi^* \right\} \tag{1.8a}$$

$$= \frac{i}{2m} \int_{\mathbb{R}^3} \mathrm{d}^3x \, \nabla_{\vec{x}} \cdot \left[\psi^* \vec{\nabla} \psi - \psi \left(\vec{\nabla} \psi^* \right) \right], \tag{1.8b}$$

where we integrated by parts[1] so we can define

$$\vec{j}(\vec{x}, t) = -\frac{i}{2m} \left(\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^* \right), \tag{1.11}$$

so that our equation now reads

$$\frac{\mathrm{d}\mathbb{P}}{\mathrm{d}t} = -\int_{\mathbb{R}^3} \mathrm{d}^3x \, \vec{\nabla}_x \cdot \vec{j} = \int_{\partial \mathbb{R}^3} \vec{j} \cdot \hat{n} \, \mathrm{d}^2x = 0, \tag{1.12}$$

since the wavefunction is integrable: that is, it goes to zero *quickly* as $|\vec{x}| \to \infty$. Therefore, $\left|\vec{j}\right| \to 0$ as $|\vec{x}| \to \infty$. For a more detailed explanation, see the Quantum Mechanics notes by Manzali [Man19, page 147].

So, if the probability is equal to one at a certain time than it keeps being equal to one.

We can express this as a differential equation for the integrand: the *continuity equation*,

$$\frac{\partial}{\partial t} \left| \psi(\vec{x}, t) \right|^2 + \vec{\nabla} \cdot \vec{j} = 0. \tag{1.13}$$

Let us now consider the way to solve the free Schrödinger equation:

$$i \frac{\partial \psi}{\partial t} = -\frac{\nabla^2 \psi}{2m}. \tag{1.14}$$

[1] The calculation, expressed using index notation (and the Einstein summation convention) for clarity, is as follows:

$$\psi^* \partial_i \partial^i \psi = \partial_i \left(\psi^* \partial^i \psi \right) - (\partial_i \psi^*)(\partial^i \psi) \tag{1.9}$$

and similarly for the other term. The terms which come out as the products of two gradients, $(\partial_i \psi^*)(\partial^i \psi)$, are equal for both the terms, so they simplify. Then, we are left with

$$\psi^* \partial_i \partial^i \psi - \psi \partial_i \partial^i \psi^* = \partial_i \left(\psi^* \partial^i \psi - \psi \partial^i \psi^* \right). \tag{1.10}$$

We start from an ansatz of the equation being factorizable: $\psi(\vec{x},t) = \chi(t)\varphi(\vec{x})$. So, we get

$$i\frac{\partial \psi_0}{\partial t} = \varphi(\vec{x}) i\frac{\partial \chi}{\partial t} \tag{1.15}$$

on the LHS, and

$$H_0(\psi) = -\chi(t)\frac{\vec{\nabla}^2}{2m}\varphi(\vec{x}) \tag{1.16}$$

on the RHS. Dividing both by $\psi = \chi\varphi$ we get

$$i\frac{1}{\chi}\frac{\partial \chi}{\partial t} = -\frac{1}{\varphi}\frac{\vec{\nabla}^2}{2m}\varphi\,, \tag{1.17}$$

and since these are dependent only on time (for the LHS) and only on position (for the RHS) they must be separately constant: let us call their value E. Therefore, we can integrate them to get

$$\frac{\partial \chi}{\partial t} = -iE\chi \implies \chi(t) = \chi(0)\exp(-iEt) \tag{1.18}$$

and

$$\nabla^2\varphi = -2mE\varphi \implies \varphi(\vec{x}) = \varphi(0)\exp\Big(i\vec{k}\cdot\vec{x}\Big)\,. \tag{1.19}$$

Here , $\vec{k}$ is a 3D vector such that $\left|\vec{k}\right|^2 = 2mE$.

This is called the *dispersion relation*. So, the full solution, which is called a *monochromatic* solution, is

$$\psi(\vec{x},t) = \exp\left(-i\Big(Et - \vec{k}\cdot\vec{x}\Big)\right), \tag{1.20}$$

where $\left|\vec{k}\right|^2 = 2mE$.

The general solution will be a continuous superposition of solutions of this form:

$$\psi(\vec{x},t) = \frac{1}{(2\pi)^{3/2}}\int \mathrm{d}^3x\,\widetilde{\varphi}(\vec{k})\,\exp\left(-i\Big(\omega_k - \vec{k}\cdot\vec{x}\Big)\right)\Big|_{\omega_k = \frac{\left|\vec{k}\right|^2}{2m}}\,. \tag{1.21}$$

Our conventions for the Fourier transform are:

$$\varphi(\vec{x}) = \frac{1}{(2\pi)^{3/2}}\int \mathrm{d}^3x\,\widetilde{\varphi}(\vec{k})\exp\Big(-i\vec{k}\cdot\vec{x}\Big)\widetilde{\varphi}(\vec{x}) \quad = \frac{1}{(2\pi)^{3/2}}\int \mathrm{d}^3x\,\varphi(\vec{k})\exp\Big(i\vec{k}\cdot\vec{x}\Big), \tag{1.22}$$

so we use the symmetric definition. Other conventions have factors $(2\pi)^{-3}$ on one side and nothing on the other; it is the same but the we must be consistent.

It is a theorem that $\left|\varphi\right|^2 = \left|\widetilde{\varphi}\right|^2$, where the square norm of φ, $\left|\varphi\right|^2$, is just the integral of $\varphi^*\varphi$ over all 3D space.

The 3D dirac delta function is defined as

$$\delta^3(\vec{x}-\vec{y}) = \frac{1}{(2\pi)^3}\int \mathrm{d}^3k \exp\left(-i\vec{k}\cdot(\vec{x}-\vec{y})\right), \tag{1.23}$$

and the 3D delta in the momentum space is perfectly analogous.

The Schrödinger equation is manifestly *non relativistic*: we started from the nonrelativistic expression $E = p^2/2m + V$, so we should expect so. In the differential equation we have a second spatial derivative and a first temporal derivative: there is no way to write such an equation covariantly.

This kind of law of physics is only invariant under *galilean transformations*, which do not change time.

Saturday 2020-3-14, compiled 2020-03-31

1.2 Conventions

1.2.1 Natural units

Two constants which often come up in theoretical physics are Planck's constant $\hbar = h/2\pi \approx 6.582 \times 10^{-22}\,\mathrm{MeV/Hz}$ and the speed of light $c \approx 2.997 \times 10^8\,\mathrm{m/s}$. They are used to convert quantities which are *equivalent*: a length is equivalent to a time interval if light passes through that length in that time interval in a vacuum; an energy is equivalent to an angular velocity if a photon with that angular velocity has that energy.

So, we can express lengths in "seconds $\times c$", energies in "kilograms times c^2" or "Hertz times $\hbar$", and so on. Since this is very convenient, we go one step further and do not write the c and the $\hbar$. This allows us to not worry about the number of times these should appear in a formula.

Formally, we do this by imposing the conditions $\hbar = c = 1$, where 1 is adimensional. Then, we can select a common unit and use it for everything: a common choice is the electronVolt (or its multiples).

Some examples of physical quantities in natural units:

1. masses and energies are both measured in eV (for masses, we should multiply by c^2);
2. linear momenta $p = mv$ are measured in eV (times c);
3. angular momenta $L = r \wedge p$ are adimensional (they could be expressed in units of $\hbar$);
4. times and lengths are both measured in eV^{-1}.

This shortens formulas, but it obscures their dimensionality. Thankfully we can always reinsert the necessary cs and $\hbar$s by dimensional analysis.

1.2.2 Relativistic notation

A contravariant vector is denoted by writing its components,

$$v^\mu = \begin{bmatrix} v^0 \\ v^1 \\ v^2 \\ v^3 \end{bmatrix}, \tag{1.24a}$$

and examples of these include the position 4-vector $x^\mu = (t, \vec{x})$, and the 4-momentum $p^\mu = (E, \vec{p})$.

We shall use the worse convention for the metric, that is, the mostly negative $(+,-,-,-)$ one. This allows us to obtain covariant vectors as

$$x_\mu = \eta_{\mu\nu} x^\nu = (t, -\vec{x})\,. \tag{1.25}$$

The derivative operator, instead, is naturally covariant:

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = (\partial_t, \vec{\nabla})\,. \tag{1.26}$$

1.3 The Klein Gordon equation

We shall use the correspondence principle, as we did for the Schrödinger equation; however this time we will apply it to a relativistic particle. Its 4-momentum has a modulus square equal to the square of its mass: M^2, since it is a relativistic invariant and we may compute it in any reference frame we like. In a generic frame, it is

$$M^2 = p^\mu p_\mu = p^\mu \eta_{\mu\nu} p^\nu = E^2 - \left|\vec{p}\right|^2, \tag{1.27}$$

which allows us to write the *dispersion relation*

$$E^2 = \vec{p}^2 + M^2\,. \tag{1.28}$$

This is *quadratic* in the energy, as opposed to the nonrelativistic expression $E = m + mv^2/2$.

Applying the correspondence principle, we find

$$-\partial_t^2 \varphi(\vec{x}, t) = \left(-\nabla^2 + M^2\right)\varphi(\vec{x}, t) \tag{1.29a}$$

$$0 = \left[\left(\partial_t^2 - \nabla^2\right) + M^2\right]\varphi(\vec{x}, t) \tag{1.29b}$$

$$= \left[\Box + M^2\right]\varphi(\vec{x}, t)\,, \tag{1.29c}$$

where we defined $\Box = \partial^\mu \partial_\mu = \partial_t^2 - \nabla^2$. Another way to see this is that, compactly stated, the correspondence principle is $p_\mu = i\partial_\mu$,[2] so from $p^2 = M^2$ we get

$$\left[\Box + M^2\right]\varphi(\vec{x}, t) = 0\,. \tag{1.30}$$

[2] So we get $E = p_0 = p^0 = i\partial_t$, while $\vec{p} = p^i = -p_i = -i\vec{\nabla} = -i\partial_i$.

This is the *free Klein-Gordon relativistic equation*.

Let us check its covariance *a posteriori*, even though it is guaranteed since we started from a covariant relation. Both $M^2 = p^\mu p_\mu$ and $\Box = \partial^\mu \partial_\mu$ are scalars.

What about the wavefunction φ? It should transform under a Lorentz transformation $x \to x' = \Lambda x$ as

$$\varphi'(x') = \varphi(x)\,. \tag{1.31}$$

This amounts to saying that it is a *scalar* function. With these constraints, we can say that the Klein-Gordon equation is *covariant*; moreover, since it is a scalar equation it is actually *invariant*. If we apply a Lorentz transformation, we find that indeed

$$\Big[\Box' + M'^2\Big]\varphi'(x') = \Big[\Box + M^2\Big]\varphi(x)\,, \tag{1.32}$$

since $\Box$, M^2 and $\varphi(x)$ are scalars; therefore covariance is proven. If this is zero in an inertial reference frame, it is also zero in any other inertial reference frame.

1.3.1 Continuity equation

Now, let us seek a probability current for the KG equation as we did with the Schrödinger equation. Let us multiply on the left the KG equation by the conjugate of the wavefunction, φ^*. We shall use this equation and its conjugate:

$$\varphi^*\Big[\Box + M^2\Big]\varphi = 0 \tag{1.33a}$$

$$\varphi\Big[\Box + M^2\Big]\varphi^* = 0\,, \tag{1.33b}$$

these both hold since $\Box$ and M^2 are real. If we subtract one of these from the other, the mass terms simplify and we get

$$0 = \varphi^*\Box\varphi - \varphi\Box\varphi^* \tag{1.34a}$$

$$= \varphi^*\partial^\mu\partial_\mu\varphi - (\varphi^* \leftrightarrow \varphi)\,, \tag{1.34b}$$

where the notation $-(\varphi^* \leftrightarrow \varphi)$ means that we are subtracting the same thing which appears before, but written swapping φ and φ^*. We can expand the derivatives:

$$0 = \partial^\mu\Big(\varphi^*\partial_\mu\varphi\Big) - \big(\partial^\mu\varphi^*\big)\Big(\partial_\mu\varphi\Big) - (\varphi^* \leftrightarrow \varphi) \tag{1.35a}$$

$$= \partial^\mu\Big(\varphi^*\partial_\mu\varphi\Big) - (\varphi^* \leftrightarrow \varphi) \tag{1.35b}$$

$$= \partial^\mu\Big(\varphi^*\partial_\mu\varphi - \varphi\partial_\mu\varphi^*\Big) \stackrel{\text{def}}{=} -2i\partial^\mu j_\mu\,, \tag{1.35c}$$

The product of the gradients is symmetric under interchange of φ and φ^*, since the metric is constant.

where we defined the 4-current

$$j_\mu = \frac{i}{2}\varphi^*\partial_\mu\varphi - (\varphi^* \leftrightarrow \varphi)\,, \tag{1.36}$$

so we can write the conservation equation $\partial^\mu j_\mu = \partial_\mu j^\mu = 0$ in 3-vector form as:

$$\partial_t \rho + \vec{\nabla} \cdot \vec{j}, \tag{1.37}$$

where

$$\rho = \frac{i}{2}\varphi^* \partial_t \varphi - (\varphi^* \leftrightarrow \varphi) \qquad \text{and} \qquad \vec{j} = -\frac{i}{2}\varphi^* \partial^i \varphi - (\varphi^* \leftrightarrow \varphi)\,. \tag{1.38}$$

Minus sign since we want the contravariant components.

We can integrate the continuity equation over all 3D space to obtain a conserved quantity:

$$\int_{\mathbb{R}^3} \mathrm{d}^3x\, \rho \overset{\text{def}}{=} Q\,, \tag{1.39}$$

which is actually constant since

$$\frac{\mathrm{d}Q}{\mathrm{d}t} = \int_{\mathbb{R}^3} \mathrm{d}^3x\, \partial_t \rho = -\int_{\mathbb{R}^3} \mathrm{d}^3x\, \vec{\nabla} \cdot \vec{j} = -\int_{S^2_\infty} \vec{j} \cdot \hat{n}\, \mathrm{d}A \to 0\,. \tag{1.40}$$

Used the divergence theorem, the surface S^2_∞ is a sphere with diverging radius.

We call this conserved quantity a "charge". There is an issue: in the Schrödinger case the quantity called ρ was positive by definition; now instead ρ and Q are not necessarily positive.

This can be proven as follows: suppose ρ was positive for a certain wavefunction φ. The conjugate wavefunction φ^* is also a solution to the KG equation, and for it the density will be negative, since permuting φ and φ^* is equivalent to changing the sign of j_μ.

So, we cannot use the Bohr ansatz, interpreting Q as a probability.

1.3.2 Solutions to the free KG equation

Let us forget about the physical interpretation for a while, and discuss the general solutions of the KG equation. We can decompose the wavefunction $\varphi(x)$ in terms of its Fourier transform $\widetilde{\varphi}(k)$:

$$\varphi(x) = \frac{1}{(2\pi)^2} \int \mathrm{d}^4k\, e^{-ik^\mu x_\mu} \widetilde{\varphi}(k)\,. \tag{1.41}$$

In order for this to be covariant, if φ is a scalar then $\widetilde{\varphi}$ also must be. The argument of the exponential is also a scalar.

The volume form in the momentum space d^4k is a scalar: under a Lorentz transformation it transforms as

$$\mathrm{d}^4k' = |\det \Lambda|\, \mathrm{d}^4k\,, \tag{1.42}$$

so it does not change since $|\det \Lambda| = 1$ for Lorentz transformations.

Claim 1.3.1. *The inverse Fourier transform reads*

$$\widetilde{\varphi}(k) = \frac{1}{(2\pi)^2} \int \mathrm{d}^4x\, e^{ik^\mu x_\mu} \varphi(x)\,. \tag{1.43}$$

Proof. We take the transform of the antitransform:

$$\widetilde{\varphi}(k) = \frac{1}{(2\pi)^2}\int \mathrm{d}^4x\,\varphi(x)e^{ik^\mu x_\mu} \tag{1.44a}$$

$$= \frac{1}{(2\pi)^4}\int \mathrm{d}^4x\,e^{ik^\mu x_\mu}\int \mathrm{d}^4k'\,e^{-ik'^\mu x_\mu}\varphi(k') \tag{1.44b}$$

$$= \int \mathrm{d}^4k'\left[\frac{1}{(2\pi)^4}\int \mathrm{d}^4x\,e^{-i(k'^\mu-k^\mu)x_\mu}\right]\varphi(k') \tag{1.44c}$$

$$= \int \mathrm{d}^4k'\,\delta^{(4)}(k-k')\varphi(k') = \varphi(k)\,, \tag{1.44d}$$

where we used the definition of the 4D Dirac δ function (here in position space, the definition in momentum space is perfectly analogous):

$$\delta^{(4)}(x^\mu) = \frac{1}{(2\pi)^4}\int \mathrm{d}^4k\,e^{-ik_\mu x^\mu}\,, \tag{1.45}$$

and its main property:

$$\int \mathrm{d}^4x\,\delta^{(4)}(x)f(x) = f(0)\,. \tag{1.46}$$

□

Now, to solve the KG equation we insert the Fourier expression of the wavefunction into it:

$$0 = \left[\Box + M^2\right]\varphi(x) = \int \frac{\mathrm{d}^4k}{(2\pi)^2}\left[-k^2+M^2\right]e^{-ik^\mu x_\mu}\widetilde{\varphi}(k)\,, \tag{1.47}$$

The $\Box$ operator acts in position space, so it has no effect on $\widetilde{\varphi}(k)$: it applies only to the exponential, yielding $-k^2 = (-ik^\mu)(-ik_\mu)$.

and since the integral must be zero the integrand must be zero as well. This is because the monochromatic waves are a basis for the Hilbert space, and the Fourier transform is an isomorphism of Hilbert spaces, which maps the zero function to the zero function.

So, we can use the ansatz $\widetilde{\varphi}(k) = \delta(k^2-M^2)\widetilde{f}(k)$, where $\widetilde{f}(k)$ is a generic scalar function. If $\widetilde{\varphi}(k)$ is written in this way, it automatically satisfies the KG equation.

Now, recall that for a Dirac delta function applied to a generic function $f(x)$, whose zeroes are enumerated by the index i (that is, $f(x_i) = 0$ for all i between 1 and N) the following property holds:

$$\delta(f(x)) = \sum_{i=1}^{N}\frac{\delta(x-x_i)}{|f'(x_i)|}\,. \tag{1.48}$$

We can apply this property to $\delta(k^2-M^2)$. First of all, since $k^2 = k_0^2 - \left|\vec{k}\right|^2$, we can write this expression as $\delta(k_0^2-\omega_k^2)$, by defining ω_k as the positive root:

$$\omega_k = +\sqrt{|k|^2+M^2}\,. \tag{1.49}$$

Now, we apply the δ function property:

$$\delta(k^2 - M^2) = \delta(k_0^2 - \omega_k^2) = \frac{\delta(k_0 - \omega_k)}{|2k_0|} + \frac{\delta(k_0 + \omega_k)}{|2k_0|} \tag{1.50a}$$

$$= \frac{\delta(k_0 - \omega_k) + \delta(k_0 + \omega_k)}{2\omega_k}\,, \tag{1.50b}$$

where we substituted $|k_0| = \omega_k$, which holds both if $k_0 = \omega_k$ and if $k_0 = -\omega_k$. This finally gives us

$$\widetilde{\varphi}(k) = \frac{1}{2\omega_k}\big(\delta(k_0 - \omega_k) + \delta(k_0 + \omega_k)\big)\widetilde{f}(k)\,, \tag{1.51}$$

which we can insert this into the Fourier transform of $\varphi(x)$:

$$\varphi(x) = \frac{1}{(2\pi)^2}\int \mathrm{d}^4k\, \widetilde{\varphi}(k) e^{-ik^\mu x_\mu} \tag{1.52a}$$

$$= \frac{1}{(2\pi)^2}\int \frac{\mathrm{d}^4k}{2\omega_k}\big(\delta(k_0 - \omega_k) + \delta(k_0 + \omega_k)\big)e^{-ik^\mu x_\mu}\widetilde{f}(k) \tag{1.52b}$$

$$= \frac{1}{(2\pi)^2}\int \frac{\mathrm{d}^3k}{2\omega_k}\Big[e^{-i\omega_k x_0}e^{i\vec{k}\cdot\vec{x}}\widetilde{f}(\omega_k, \vec{k}) + e^{i\omega_k x_0}e^{i\vec{k}\cdot\vec{x}}\widetilde{f}(-\omega_k, \vec{k})\Big] \tag{1.52c}$$

We integrate in $\mathrm{d}k^0$ to get rid of the δ functions.

$$= \frac{1}{(2\pi)^2}\int \frac{\mathrm{d}^3k}{2\omega_k}\Big[e^{-ik^\mu x_\mu}\widetilde{f}(k^\mu) + e^{ik^\mu x_\mu}\widetilde{f}(-k^\mu)\Big]_{k_0=\omega_k}\,, \tag{1.52d}$$

where we indicate $k^\mu\big|_{k_0=\omega_k} = (\omega_k, \vec{k})$.

We used the fact that, in the Fourier transform integral, the terms $e^{i\vec{k}\cdot\vec{x}}\widetilde{f}(\vec{x})$ and $e^{-i\vec{k}\cdot\vec{x}}\widetilde{f}(-\vec{x})$ are equivalent: this is because, since we are integrating over all of 3D space, any contributions which are *odd* in $\vec{k}$ will not affect the total integral, therefore we can only consider the even part of the integrand.

Now, in order to simplify the notation we define

$$a(k) = \frac{\widetilde{f}(k)}{\sqrt{2\pi}\sqrt{2\omega_k}} \qquad \text{and} \qquad b(k) = \frac{\widetilde{f}(-k)}{\sqrt{2\pi}\sqrt{2\omega_k}}\,, \tag{1.53}$$

which are arbitrary like the initial function $\widetilde{f}$, however they are connected since $a(k) = b^*(-k)$. So, the final solution reads:

$$\varphi(x) = \frac{1}{(2\pi)^{3/2}}\int \frac{\mathrm{d}^3k}{\sqrt{2\omega_k}}\Big[a(k)e^{-ik\cdot x} + b^*(k)e^{ik\cdot x}\Big]_{k_0=\omega_k} \tag{1.54a}$$

$$= \varphi_+(x) + \varphi_-(x)\,. \tag{1.54b}$$

Recall that all ks appearing in the expression are to be interpreted as $(\omega_k, \vec{k})$. The part dependent on $a(k)$ is conventionally called the *positive energy* solution φ_+, while the part depending on $b^*(k)$ is the *negative energy* solution φ_-.

This is because, as the energy of a wavefunction φ is computed by $E = i\partial_t\varphi$, we have

$$E(\varphi_+) = i\partial_0\left\{\frac{1}{(2\pi)^{3/2}}\int \frac{\mathrm{d}^3k}{\sqrt{2\omega_k}}a(k)e^{-ik^\mu x_\mu}\right\} = i(-i)\omega_k\varphi_+ = \omega_k\varphi_+ \tag{1.55a}$$

$$E(\varphi_-) = i\partial_0 \left\{ \frac{1}{(2\pi)^{3/2}} \int \frac{\mathrm{d}^3 k}{\sqrt{2\omega_k}} b^*(k) e^{ik^\mu x_\mu} \right\} = i(i)\omega_k \varphi_- = -\omega_k \varphi_- \,, \tag{1.55b}$$

so φ_+ has a positive energy while φ_- has a negative one.

This is the main difference between the Schrödinger and KG equations.

The solution to the KG equation is not explicitly covariant, but all the steps preserved covariance so the final solution is still covariant.

The KG equation is real, since $\Box$ is a real operator and M^2 is real, so it will admit real solutions. In order to find these we impose $\varphi = \varphi^*$.

Claim 1.3.2. *$\varphi = \varphi^*$ implies $a = b$.*

Proof. We write only the argument of the integrals for simplicity:

$$\varphi \sim a e^{-ikx} + b^* e^{ikx} \tag{1.56a}$$

$$\varphi^* \sim a^* e^{ikx} + b e^{-ikx} \,, \tag{1.56b}$$

so if $\varphi = \varphi^*$ we must identify these component by component, so we must have $a = b$, and $a^* = b^*$. □

Then, the most general real solution to the KG equation is

$$\varphi_{\mathbb{R}}(x) = \frac{1}{(2\pi)^{3/2}} \int \frac{\mathrm{d}^3 k}{\sqrt{2\omega_k}} \left[a(k) e^{-ik\cdot x} + a^*(k) e^{ik\cdot x} \right]_{k_0 = \omega_k} . \tag{1.57}$$

Claim 1.3.3. *For a real KG solution, the function $a(k)$ can be written as*

$$a(k) = \frac{1}{(2\pi)^{3/2}} \int \frac{\mathrm{d}^3 x}{\sqrt{2\omega_k}} \left(\omega_k \varphi(x) + i\partial_0 \varphi(x) \right) e^{ik\cdot x} \Big|_{k_0 = \omega_k} . \tag{1.58}$$

Proof. The solution is found by direct substitution of $\varphi_{\mathbb{R}}$ into the expression for a in order to verify it; the operations are all reversible so we can use the derivation backwards or forwards equivalently. We find

$$a \overset{?}{=} \frac{1}{(2\pi)^3} \int \frac{\mathrm{d}^3 k \, \mathrm{d}^3 x}{2\omega_k} \left[\omega_k \left(a e^{-ik\cdot x} + a^* e^{ik\cdot x} \right) + i\partial_0 \left(a e^{-ik\cdot x} + a^* e^{ik\cdot x} \right) \right] e^{ik\cdot x} \Big|_{k_0 = \omega_k} \tag{1.59a}$$

$$= \frac{1}{(2\pi)^3} \int \frac{\mathrm{d}^3 k \, \mathrm{d}^3 x}{2\omega_k} \left[\left(\omega_k + i(-ik_0) \right) a^{-ik\cdot x} + \left(\omega_k + i(ik_0) \right) a^* e^{ik\cdot x} \right] e^{ik\cdot x} \Big|_{k_0 = \omega_k} \tag{1.59b}$$

$$= \frac{1}{(2\pi)^3} \int \frac{\mathrm{d}^3 k \, \mathrm{d}^3 x}{2\omega_k} \left[2\omega_k a^{-ik\cdot x} \right] e^{ik\cdot x} \Big|_{k_0 = \omega_k} \tag{1.59c}$$

Used the fact that $\omega_k = k_0$, and $i^2 = -1$.

$$= \frac{1}{(2\pi)^{3/2}} \int \mathrm{d}^3 x \, e^{i\vec{k}\cdot\vec{x}} \left[\frac{1}{(2\pi)^{3/2}} \int \mathrm{d}^3 k \, e^{-i\vec{k}\cdot\vec{x}} a \right] = a \,. \tag{1.59d}$$

3D Fourier inverse and direct transform.

We simplified two factors of $e^{ik_0 x^0}$ and $e^{-ik_0 x^0}$ since they are equal everywhere ($k_0 = \omega_k$).

□

Claim 1.3.4. *For a complex KG solution, the functions $a(k)$ and $b^*(k)$ can be written as*

$$a(k) = \frac{1}{(2\pi)^{3/2}} \int \frac{\mathrm{d}^3x}{\sqrt{2\omega_k}} \left(\omega_k \varphi(x) + i\partial_0 \varphi(x)\right) e^{ik\cdot x}\Big|_{k_0=\omega_k} \tag{1.60a}$$

$$b^*(k) = \frac{1}{(2\pi)^{3/2}} \int \frac{\mathrm{d}^3x}{\sqrt{2\omega_k}} \left(\omega_k \varphi(x) - i\partial_0 \varphi(x)\right) e^{-ik\cdot x}\Big|_{k_0=\omega_k} . \tag{1.60b}$$

Proof. The derivation is the same as the real-valued solution case. The b^* terms simplify if there is a plus in front of the $i\partial_0$ term, if instead we have a minus the a terms simplify; everything else is precisely the same. □

Claim 1.3.5. *Given two real solutions to the KG equation, φ_1 and φ_2, one can always write a complex solution $\varphi = (\varphi_1 + i\varphi_2)/\sqrt{2}$.*

Then, the functions a and b^* for the complex solution can be written in terms of the a_1 and a_2 for the real solution as:

$$a = \frac{a_1 + ia_2}{\sqrt{2}} \tag{1.61a}$$

$$b = \frac{a_1 - ia_2}{\sqrt{2}} . \tag{1.61b}$$

Proof. We write out the complex function:

$$\frac{\varphi_1 + i\varphi_2}{\sqrt{2}} = \frac{1}{(2\pi)^{3/2}} \int \frac{\mathrm{d}^3k}{\sqrt{2\omega_k}} \left[\frac{a_1 + ia_2}{\sqrt{2}} e^{-ik\cdot x} + \frac{a_1^* + ia_2^*}{\sqrt{2}} e^{ik\cdot x}\right] , \tag{1.62}$$

so, since $b^* = \left(a_1^* + ia_2^*\right)/\sqrt{2}$, we can get b by conjugating,

$$b = \frac{a_1 - ia_2}{\sqrt{2}} , \tag{1.63}$$

while a can be directly read off the expression. □

Monday 2020-3-16, compiled 2020-03-31

1.3.3 The Klein-Gordon equation in the presence of an external electromagnetic field

A complex scalar solution to the Klein-Gordon equation can represent a charged relativistic spin-0 particle. Since the particle is charged, it is interesting to study its interaction with the electromagnetic field.

We will discuss only the interaction of the particle with an externally determined field, that is, we will not discuss how the particle influences the field around it.

In order to describe the electric and magnetic fields in a covariant way we use the four-vector $A_\mu = (A_0, \vec{A})$, such that $\vec{E} = -\vec{\nabla} A_0 - \partial_0 \vec{A}$ and $\vec{B} = \vec{\nabla} \times \vec{A}$, or, in covariant terms,

$$F^{\mu\nu} = 2\partial^{[\mu} A^{\nu]} , \tag{1.64}$$

where the antisymmetric field-strength tensor $F^{\mu\nu}$ encodes both the electric and magnetic fields.

Definition 1.3.1. *The **minimal coupling** to an external electromagnetic field is obtained by substituting in the wave equation the partial derivative ∂_μ with the* covariant derivative

$$\mathrm{D}_\mu \overset{def}{=} \partial_\mu + iqA_\mu\,, \tag{1.65}$$

where q is the electric charge of the particle.

Inserting this, the coupled Klein-Gordon equation reads

$$\left[\mathrm{D}^\mu \mathrm{D}_\mu + M^2\right]\varphi(x) = 0\,. \tag{1.66}$$

Recall that the momentum is defined as $p_\mu = i\partial_\mu$, so this substitution is equivalent to changing the momentum to $i(\partial_\mu + iqA_\mu) = p_\mu - qA_\mu$.

This is the same minimal coupling ansatz which is used in nonrelativistic quantum mechanics: there, the minimally-coupled Schrödinger equation reads

$$E\psi = \left[\frac{\left(\vec{p} - q\vec{A}\right)^2}{2M} + qA_0\right]\psi\,, \tag{1.67}$$

in which we can see the two contributions: the three-momentum $\vec{p}$ is exchanged for $\vec{p} - q\vec{A}$, while the energy E is exchanged for $E - qA_0$ (and the term is brought on the other side of the equation for convenience).

Let us make the terms in the minimally coupled Klein-Gordon equation explicit:

$$\left[\left(\partial^\mu + iqA^\mu\right)\left(\partial_\mu + iqA_\mu\right) + M^2\right]\varphi = 0 \tag{1.68a}$$

$$\left[\Box + iqA^\mu\partial_\mu + iq\partial_\mu A^\mu - q^2A^2 + M^2\right]\varphi = 0 \tag{1.68b}$$

$$\left[\Box + 2iqA^\mu\partial_\mu + iq\left(\partial_\mu A^\mu\right) - q^2A^2 + M^2\right]\varphi = 0\,, \tag{1.68c}$$

Do note that anything on the right acts on anything on the left: the application of the derivatives looks like $\mathrm{D}^\mu\left(\mathrm{D}_\mu(\varphi)\right)$. So, the term $\partial_\mu A^\mu$ should be read as $\partial_\mu\left(A^\mu\varphi\right)$, which we expanded into $\left(\partial_\mu A^\mu\right) + A^\mu\partial_\mu$ — all acting on φ, but the term $\left(\partial_\mu A^\mu\right)$ is just multiplied by φ, it does not perform a differentiation.

The Coulomb potential

The 4-potential is not physical: if we change it by $A_\mu \to A'_\mu = A_\mu + \partial_\mu\Lambda$ for some scalar function Λ it does not change the resulting measurable electric and magnetic fields. Therefore, while still retaining full generality in our description of physical systems we can impose certain conditions, such as $\partial_\mu A^\mu = 0$. This condition, known as the *Coulomb gauge*, does not actually fix all of the gauge freedom — that is, even by imposing this we still do not have a one-to-one correspondence between the physical fields and the 4-potentials: after

imposing it, we can still perform gauge transformations where the function Λ is harmonic, that is, it satisfies $\Box\Lambda = 0$.

This condition is convenient since it allows us to get rid of a term in the KG equation, so we impose it.

Antimatter: an interpretation for the negative-energy solution

Let us consider a simple case: the monochromatic solution to the KG equation, $\varphi_{\pm}(x) = e^{\mp ik\cdot x}$, coupled to the EM field. Let us suppose that the 4-momentum $k^\mu = (\omega_k, \vec{k})$ corresponding to the two solutions is fixed, that is, the positive energy solution has $E\varphi^+ = \omega_k$ while the negative energy solution has $E\varphi^- = -\omega_k$, with the same ω_k and the same $\vec{k}$.

Splitting the energy and momentum terms, the equation reads:

$$\left[\left(E - qA_0\right)^2 + \left(\vec{p} - q\vec{A}\right) + M^2\right]\varphi^{\pm}(x) = 0\,, \tag{1.69}$$

where $E = i\partial_t$ while $\vec{p} = -i\vec{\nabla}$.

Then, we can write the two equations like

$$\left[\left(\omega_k - qA_0\right)^2 + \left(\vec{k} - q\vec{A}\right) + M^2\right]\varphi^{+}(x) = 0 \tag{1.70a}$$

$$\left[\left(\omega_k + qA_0\right)^2 + \left(\vec{k} + q\vec{A}\right) + M^2\right]\varphi^{-}(x) = 0\,, \tag{1.70b}$$

where we used the fact that $(-\omega_k - qA_0)^2 = (\omega_k + qA_0)^2$, and similarly for the other term.

So, we can see that the two equations can be transformed into each other also by swapping the charge, $q \to -q$.

The interpretation for this is that the KG equation describes two degrees of freedom, which we call a *particle* (with $E > 0$) and an *antiparticle* (with $E < 0$).

The particle and antiparticle have the same mass, but their charge is opposite. In a certain sense, the existence of antimatter is a prediction of relativistic quantum mechanics.

1.3.4 The nonrelativistic limit

As a consistency check for our relativistic equation, we wish to verify that the nonrelativistic limit of the KG equation is the Schrödinger equation.

In the nonrelativistic limit the mass of the particle M is much larger than its momentum p, so we can expand:

$$E = \sqrt{|p|^2 + M^2} = M\sqrt{1 + \frac{|p|^2}{M^2}} = M + \underbrace{\frac{|p|^2}{2M}}_{E_k} + \mathcal{O}\left(\frac{|p|^4}{M^3}\right). \tag{1.71}$$

In quantum mechanics the time evolution of a particle depends on its energy, so if $M \gg E_k$ the evolution due to the mass will be much faster than that due to the kinetic energy: so, we factor it out by

$$\varphi(t, \vec{x}) = e^{-iMt}\varphi'(t, \vec{x})\,, \tag{1.72}$$

where the evolution of φ' will look like $e^{-iE_k t}\varphi'$.

Now, let us expand the derivative terms in the KG equation (in the Coulomb gauge, so we do not worry about $\partial_\mu A^\mu$):

$$\begin{aligned} \mathrm{D}^\mu \mathrm{D}_\mu &= \left(\partial^0 + iqA^0\right)\left(\partial_0 + iqA_0\right) + \left(\partial^i + iqA^i\right)\left(\partial_i + iqA_i\right) && \text{(1.73a)} \\ &= \left(\partial_0 + iqA_0\right)^2 - \left(\partial_i + iqA_i\right)^2 && \text{(1.73b)} \\ &= \left(\partial_0 + iqA_0\right)^2 - \left(\vec{\nabla} - iq\vec{A}\right)^2, && \text{(1.73c)} \end{aligned}$$

where we used the fact that $\vec{A} = A^i$, while $\vec{\nabla} = \partial_i = -\partial^i$.

In the full KG equation applied to the decomposed field $\varphi = e^{-iMt}\varphi'$ we move the momentum terms to the right and keep the mass and energy on the left:

$$\left[\left(\partial_0 + iqA_0\right)^2 + M^2\right] e^{-iMt}\varphi' = \left(\nabla - iq\vec{A}\right)^2 e^{-iMt}\varphi' \qquad \text{(1.74a)}$$

$$\left[\partial_0^2 + 2iqA_0\partial_0 - q^2A_0^2 + M^2\right] e^{-iMt}\varphi' = e^{-iMt}\left(\nabla - iq\vec{A}\right)^2\varphi'. \qquad \text{(1.74b)}$$

The term e^{-iMt} is constant with respect to the spatial coordinates

The time-derivative on the right acts both on the mass term and on the wavefunction φ'. So, we get[3]

$$e^{-iMt}\left(\nabla - iq\vec{A}\right)^2\varphi' =$$

$$= e^{-iMt}\left[\partial_0^2 - M^2 - 2iM\partial_0 + 2iqA_0(-iM) + 2iq(\partial_0 A_0) + 2iqA_0\partial_0 - q^2A_0^2 + M^2\right]\varphi' \qquad \text{(1.77a)}$$

$$= \left[\partial_0^2 - 2iM\partial_0 + 2qA_0M + 2iq(\partial_0 A_0) + 2iqA_0\partial_0 - q^2A_0^2\right]\varphi' = \left(\nabla - iq\vec{A}\right)^2\varphi', \qquad \text{(1.77b)}$$

and now we must discuss which terms we can discard.

On the right hand side we have terms of the order of the mass and ones of the order of the energy: we wish to keep only the former, since as we assumed they dominate the latter. Specifically, terms without explicit dependence on the mass are of the order of the kinetic

[3] It is really easy when doing these computations to forget some terms. A way I've found helpful is to write down the full expression,

$$\left(\partial_0 + iqA_0\right)\left(\partial_0 + iqA_0\right)\left(e^{-iMt}\varphi'\right), \qquad \text{(1.75)}$$

give binary labels (000, 001... until 111) to each term and work through all 2^3 of them. Notice the expansion of the term

$$\partial_0\partial_0\left(e^{-iMt}\varphi'\right) = \partial_0\left(-iMe^{-iMt}\varphi' + e^{-iMt}\partial_0\varphi'\right) = -iMe^{-iMt}\partial_0\varphi' - M^2e^{-iMt}\varphi' + e^{-iMt}\partial_0^2\varphi - iMe^{iMt}\varphi'. \qquad \text{(1.76)}$$

energy:[4] then, we remove and get precisely the minimally coupled Schrödinger equation:

$$\left[-2iM\partial_0 + 2q_0A_0M\right]\varphi' = \left(\vec{\nabla} - iq\vec{A}\right)^2\varphi' \tag{1.78a}$$

$$i\partial_0\varphi' = \left[-\frac{\left(\vec{\nabla} - iq\vec{A}\right)^2}{2M} + q_0A_0\right]\varphi' \,. \tag{1.78b}$$

This is precisely the equation we wrote above: the nonrelativistic Schrödinger equation for a charged spin-0 particle in an electromagnetic field.

1.3.5 Summary

1. The dispersion relation $E^2 = p^2 + m^2$ is a quadratic relation, the positive root is called $\omega_p = \sqrt{p^2 + m^2}$ and the energy can be $E = \pm\omega_p$.
2. A solution to the KG equation has two independent terms φ^+ and φ^-, which can be interpreted as a particle-antiparticle pair, where φ^+ has charge q while φ^- has charge $-q$.

   An antiparticle has the same quantum numbers, but the opposite charge.
3. There is no way to define a conserved (positive definite) probability for the KG equation, but the nonrelativistic limit of the KG equation is consistent with nonrelativistic quantum mechanics.

Claim 1.3.6. *The continuity equation for the coupled KG equation is given by*

$$\partial_\mu j^\mu_{EM} = 0 \,, \tag{1.79}$$

where

$$j^\mu_{EM} = \frac{1}{2}\left(i\varphi^*\partial^\mu\varphi - qA^\mu\varphi^*\varphi\right) - c.\ c.\,. \tag{1.80}$$

Proof. Similarly to what was done before, we notice that

$$\varphi^*\left(\mathrm{D}^\mu\mathrm{D}_\mu + M^2\right)\varphi = \varphi^*\left[\Box + 2iqA^\mu\partial_\mu + iq\left(\partial_\mu A^\mu\right) - q^2A^2 + M^2\right]\varphi = 0 \tag{1.81}$$

can be added to the negative of its complex conjugate, which reads

$$\varphi\left[\Box - 2iqA^\mu\partial_\mu - iq\left(\partial_\mu A^\mu\right)\right]\varphi^* = 0 \,, \tag{1.82}$$

[4] This is imprecise, we can do better: we distinguish the terms with time derivatives and those without. Those with time derivatives are applied to φ', which by construction evolves with $\omega = E_k$, therefore they are negligible. The other terms are $q^2A_0^2$, which is the electric potential energy, and $2iq\partial_0A_0$, which is proportional to the electric field: we assume the electric field to be nonrelativistic, that is, of intensity comparable to the kinetic energy of the particle, and much smaller than its mass.

to yield

$$0 = \varphi^*\Box\varphi + 2iqA_\mu\varphi^*\partial^\mu\varphi + iq\left(\partial_\mu A^\mu\right)\varphi\varphi^* + \\ - \varphi\Box\varphi^* + 2iqA_\mu\varphi\partial^\mu\varphi^* + iq\left(\partial_\mu A^\mu\right)\varphi\varphi^* \tag{1.83a}$$

The q^2A^2 and M^2 terms cancel since they are real

$$= \partial^\mu\left(\varphi^*\partial_\mu\varphi - \varphi\partial_\mu\varphi^*\right) + 2iq\left[A_\mu\left(\varphi^*\partial^\mu\varphi + \varphi\partial^\mu\varphi^*\right) + \varphi\varphi^*\partial_\mu A^\mu\right] \tag{1.83b}$$

$$= \partial^\mu\left[\varphi^*\partial_\mu\varphi - \varphi\partial_\mu\varphi^* + 2iqA_\mu\varphi\varphi^*\right], \tag{1.83c}$$

so the expression inside the brackets is the conserved current, up to a multiplicative factor of $i/2$. □

1.3.6 The Klein paradox

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The fact that it was not possible to derive a conserved charge for the KG equation is not just a mathematical inconvenience: we will use a gedankenexperiment to show the physical consequences of this.

Consider the scattering of a particle, which is described by a pure plane wave, on a an electromagnetic potential step. Suppose we are in a frame in which $qA^\mu = (V(x), \vec{0})$; if we are not in such a frame we can always perform a boost so that we are. Also suppose that the potential looks like a step: $V(x) = V_0[x \geq 0]$. Here "x" refers to a 1d spatial coordinate.

Now, suppose that we have an incoming wave with energy ω and momentum k_x in the $x < 0$ region. Upon impact, there will in general be a reflected wave in the $x < 0$ region and a transmitted wave in the $x > 0$ region. We will call the former φ_1 and the latter φ_2.

We can decompose both of these into a time and space exponential: $\varphi_i(t, x) = e^{-i\omega t}\chi_i(x)$, for $i = 1, 2$.

Now, the incoming wave contributes to the global wavefunction with an exponential $e^{ik_x x}$ in the $x < 0$ region. In the same region we can find the reflected wave, which has the opposite momentum; also, its amplitude is less than that of the incoming wave. We write its contribution to χ_1 as $re^{-ik_x x}$, where r is the reflection coefficient.

By a similar reasoning, in the $x > 0$ region we will have a contribution $te^{ik'_x x}$: the direction of propagation is the same as the incoming wave, the momentum might be different. In the end, our wavefunction looks like

$$\varphi(t, x) = \varphi_1[x \leq 0] + \varphi_2[x \geq 0] \tag{1.84a}$$

$$= e^{-i\omega t}\left[\chi_1[x \leq 0] + \chi_2[x \geq 0]\right] \tag{1.84b}$$

$$= e^{-i\omega t}\left[\left(e^{ik_x x} + re^{-ik_x x}\right)[x \leq 0] + te^{ik'_x x}[x \geq 0]\right]. \tag{1.84c}$$

This wavefunction will need to satisfy the KG equation everywhere, however the equation has a different form in the two regions: if $\mathrm{D}^\mu = \partial^\mu + iqA^\mu$, then we can say that the two equations are

$$\left[\partial^\mu\partial_\mu + M^2\right]\varphi_1 = 0 \tag{1.85a}$$

$$\left[\mathrm{D}^\mu \mathrm{D}_\mu + M^2\right]\varphi_2 = 0\,, \tag{1.85b}$$

so we can insert the solutions into the equations: for the region without potential we get

$$\left[\partial^\mu\partial_\mu + M^2\right]\varphi_1 = \left[+\partial_0^2 - \partial_x^2 + M^2\right]\left[e^{-i\omega t}\left(e^{ik_x x} + re^{-ik_x x}\right)\right] \tag{1.86a}$$

$$= (-i\omega)^2\varphi_1 + M^2\varphi_1 - e^{-i\omega t}\partial_x^2\left(e^{ik_x x} + re^{-ik_x x}\right) \tag{1.86b}$$

$$= -\omega^2\varphi_1 + M^2\varphi_1 - e^{-i\omega t}\left((ik_x)^2 e^{ik_x x} + r(-ik_x)^2 e^{-ik_x x}\right) \tag{1.86c}$$

$$= \left[-\omega^2 + M^2 + k_x^2\right]\varphi_1\,, \tag{1.86d}$$

notice that even though the function has components with momentum in either direction it still is an eigenfunction of the operator $\Box$! For the other region we can use the fact we discussed earlier: with the minimal substitution, the momentum becomes $p^\mu = i\partial^\mu \to i\mathrm{D}^\mu = p^\mu - qA^\mu$, so in our case we will have $p^0 \to \omega_k - qA^0 = \omega_k - V_0$, while $p^i \to \vec{k}'$, since $\vec{A} = 0$. We can substitute the energy directly since the potential is constant, so there is no $\partial_0 V_0$ term. Then, the rest of the calculation is perfectly analogous, with k'_x instead of k_x.

So, we have the two relations

$$-\omega_k^2 + k_x^2 + M^2 = 0 \qquad \text{and} \qquad -\left(\omega_k - V_0\right)^2 + k_x'^2 + M^2 = 0\,. \tag{1.87}$$

We choose the solutions in which the wave is propagating towards increasing x: so we get

$$k_x = \sqrt{\omega_k^2 - M^2} \qquad \text{and} \qquad k'_x = \sqrt{\left(\omega_k - V_0\right)^2 - M^2}\,. \tag{1.88}$$

Now we must make these consistent with each other, by imposing that at the border the function be $\mathcal{C}^1$.

Why do we fix only the first derivative? Probably something to do with the fact that the KG eq is second order, so we would need $\Box = \mathrm{D}^\mu\mathrm{D}_\mu$ at the boundary, which cannot be the case.

We can work with the spatial components χ_i, since the time evolution factors. So, for continuity we get that $\chi_1(0) = \chi_2(0)$ implies:

$$1 + r = t\,, \tag{1.89}$$

while for differentiability we get that $\partial_x\chi_1(0) = \partial_x\chi_2(0)$ implies:

$$ik_x - rik_x = itk'_x \implies \frac{k'_x}{k_x} = \frac{1-r}{t}\,. \tag{1.90}$$

Now, what do we know of these variables? Well, from the dispersion relations if we fix the mass M, the energy ω and the potential V_0 we have k_x and k'_x. Then, from the two equations we have found we can calculate r and t; their expressions are exactly those found in the nonrelativistic case. Since $1 - r = 2 - t$ we have

$$\frac{k'_x}{k_x} = \frac{2}{t} - 1 \implies \frac{k'_x + k_x}{k_x} = \frac{2}{t} \implies t = \frac{2k_x}{k'_x + k_x} \qquad \text{and} \qquad r = t - 1 = \frac{k_x - k'_x}{k'_x + k_x}\,. \tag{1.91}$$

Now, we shall discuss the probability currents for the two regions: the formula is always

$$j^\mu = \frac{i}{2}\varphi^* \partial^\mu \varphi + \frac{q}{2} A^\mu \varphi^* \varphi + \text{c. c.}\,, \tag{1.92}$$

but in the first region the potential is identically zero.

One non-obvious thing to consider is that, in general, we could have k'_x be either real or imaginary, since while $\omega^2 - M^2$ must be > 0 there is no such constraint on $(\omega - V_0)^2 - M^2$. If we conjugate an exponential as $\left(e^{iz}\right)^*$, the result is e^{-iz^*} for a general complex z. The calculation is as follows:

$$\rho_1 \overset{\text{def}}{=} j^0_{(1)} = \frac{i}{2} e^{i\omega t} \partial^0 e^{-i\omega t} |\chi_1|^2 + \text{c. c.} = \frac{2}{2}\omega |\chi_1|^2 \tag{1.93a}$$

$$j_1 \overset{\text{def}}{=} j^x_{(1)} = -\frac{i}{2}\left(e^{ik_x x} + re^{-ik_x x}\right)\partial_x \left(e^{ik_x x} + re^{-ik_x x}\right) + \text{c. c.} \tag{1.93b}$$

$$= -\frac{2}{2} i(ik_x)\left(e^{ik_x x} + re^{-ik_x x}\right)\left(e^{ik_x x} - re^{-ik_x x}\right) = k_x\left(1 - |r|^2\right) \tag{1.93c}$$

The χ_1 is not time-dependent, we get two terms by adding the conjugate. We get a minus sign from lowering the index

$$\rho_2 \overset{\text{def}}{=} j^0_{(2)} = \frac{i}{2} t^* e^{i\omega t} e^{-ik'^*_x x} t(-i\omega) e^{-i\omega t} e^{ik'_x x} + \frac{1}{2} V_0 \varphi^* \varphi + \text{c. c.} \tag{1.93d}$$

$$= (\omega - V_0)|t|^2 e^{i\left(k'_x - k'^*_x\right)x} \tag{1.93e}$$

$$j_2 \overset{\text{def}}{=} j^x_{(2)} = -\frac{i}{2} t^* e^{i\omega t} e^{-ik'^*_x x} (ik'_x) e^{-i\omega t} e^{ik'_x x} + \text{c. c.} \tag{1.93f}$$

$$= \frac{1}{2}|t|^2 e^{i\left(k'_x - k'^*_x\right)x} k'_x + \text{c. c.} \tag{1.93g}$$

$$= \frac{k'_x + k'^*_x}{2}|t|^2 e^{i\left(k'_x - k'^*_x\right)x}\,. \tag{1.93h}$$

We can define the reflection and transmission coefficients, which are probabilities:

$$\mathcal{R} = \frac{j_{\text{in}} - j_1}{j_{\text{in}}} = |r|^2 \qquad \text{and} \qquad \mathcal{T} = \frac{j_2}{j_{\text{in}}} = \frac{k'_x + k'^*_x}{2k_x}|t|^2 e^{i(k'_x - k'^*_x)x}\,, \tag{1.94}$$

where $j_{\text{in}} = k_x$ is the current density corresponding to the incoming wave alone: it is calculated as the current density we would measure in region 1 if we did not have the reflected wave component:

$$j_{\text{in}} \overset{\text{def}}{=} j^x_{(1)}\Big|_{\chi_1 = e^{ik_x x}} = -\frac{i}{2}\left(e^{ik_x x}\right)\partial_x\left(e^{ik_x x}\right) + \text{c. c.} \tag{1.95a}$$

$$= -\frac{2}{2} i(ik_x) e^{ik_x x} e^{ik_x x} = k_x\,. \tag{1.95b}$$

Now, we have three possible cases for the behavior of k'_x: it is

1. real if $\omega_k - M > V_0$: this is the nonrelativistic case;
2. imaginary if $|\omega_k - V_0| < M$: this is the intermediate case;
3. real again if $\omega_k + M < V_0$: this is the fully relativistic case.

This is shown in figure 1.1. The NR approximation can only be applied in the first case, and in the second case only as long as $V_0 < \omega_k$: the case $\omega_k - M < V_0 \ll \omega_k$ is nonrelativistic quantum tunneling.

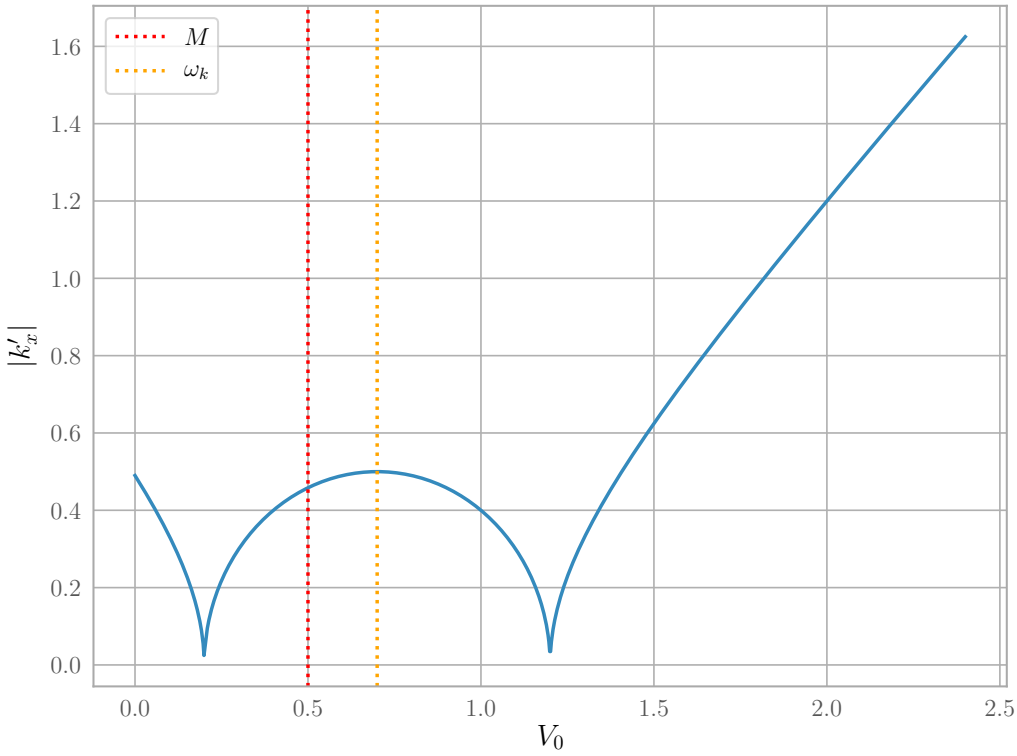

Figure 1.1: An illustration of how k'_x changes as V_0 increases. We have fixed the mass M and the the energy ω_k to 0.5 and 0.7 respectively. The regions are separated by the critical points of $|k'_x|$, at $V_0 = 0.2$ and $V_0 = 1.2$ respectively. Do note that this is a plot of the *absolute value* of k'_x: in the intermediate region it is purely imaginary.

Nonrelativistic case

Now, k_x and k'_x are both real, so $k'_x = k'^*_x$, which means that the probability currents read:

$$\rho_1 = \omega|\chi_1|^2 \qquad j_1 = k_x\left(1 - |r|^2\right) \tag{1.96a}$$

$$\rho_2 = (\omega - V_0)|t|^2 \qquad j_2 = k'_x|t|^2\,, \tag{1.96b}$$

and, since r and r are both (real and) < 1 these quantities are all positive. Also, we must have $k'_x < k_x$, so the quantities

$$\mathcal{R} = |r|^2 \qquad \text{and} \qquad \mathcal{T} = \frac{k'_x}{k_x}|t|^2 \tag{1.97}$$

are both < 1. So, it will be consistent if we impose (?) a probabilistic Born-like interpretation in which these coefficients are reflection and transmission probabilities, with $\mathcal{R} + \mathcal{T} = 1$.

Intermediate case

Now, we have $|\omega_k - V_0| < M$, so, while $k_x > 0$,

$$k'_x = \pm i\sqrt{M^2 - (\omega_k - V_0)^2}\,. \tag{1.98}$$

In principle we could have both $+$ or $-$, but we select the positive imaginary because it is the physical in which the wave travels rightward.

Now, in our computation of the probability density ρ_2 we will have a factor

$$\exp\big(i(k'_x - k'^*_x)x\big) = \exp\Big(\pm 2i^2|k'_x|x\Big) = \exp\Big(\mp 2|k'_x|x\Big)\,, \tag{1.99}$$

while for the probability current j_2 we will get a factor $k'_x + k'^*_x = 0$ multiplying everything.

So, in the end we get

$$\rho_1 = \omega|\chi_1|^2 \qquad j_1 = k_x\Big(1 - |r|^2\Big) \tag{1.100a}$$

$$\rho_2 = (\omega - V_0)|t|^2 e^{-2|k'_x|x} \qquad j_2 = 0\,. \tag{1.100b}$$

Notice that in the intermediate region we can have both $V_0 < \omega_k$ and $V_0 > \omega_k$.

In this case, we get for the reflection and transmission probabilities

$$\mathcal{R} = |r|^2 = \left|\frac{k_x - ik'_x}{k_x + ik'_x}\right| = \left|\frac{z}{z^*}\right|^2 = 1\,, \tag{1.101}$$

The ratio of z and z^* is only a phase

while $\mathcal{T} \propto j_2 = 0$.

So, in this case the particle is certainly reflected; this is compatible with the probabilistic interpretation $\mathcal{R} + \mathcal{T} = 1$. However, ρ_2 is not positive defined so it cannot be interpreted as a probability density in general.

If $V_0 < \omega_k$ we still get the vanilla-QM result of $\rho_2 \sim e^{-2|k'_x|x}$: the particle penetrates the classically forbidden region. This effect is suppressed as V_0 increases.

Fully relativistic case

This is the situation which is completely outside the realm of classical QM description, in which we expect to see relativistic effects. We have $V_0 > \omega_k + M$.

Now

$$k'_x = \pm\sqrt{(\omega_k - V_0)^2 - M^2} \in \mathbb{R}\,, \tag{1.102}$$

so the densities are

$$\rho_1 = \omega|\chi_1|^2 \qquad j_1 = k_x\Big(1 - |r|^2\Big) \tag{1.103a}$$

$$\rho_2 = (\omega - V_0)|t|^2 < 0 \qquad j_2 = k'_x|t|^2\,, \tag{1.103b}$$

where the sign of j_2 is determined by that of k'_x, which is not necessarily positive. Actually, it must be negative: to see this, we can calculate the group velocity, which would be the global

velocity of the wavepacket we are approximating. We can calculate ω_k from the dispersion relation (1.87) to get

$$v_G = \frac{\partial \omega_k}{\partial k'_x} = \frac{\partial}{\partial k'_x}\left(V_0 + \sqrt{k'^2_x + M^2}\right) = \frac{k'_x}{\sqrt{k'^2_x + M^2}} = \frac{k'_x}{\omega_k - V_0}\,, \tag{1.104}$$

where we used the dispersion relation again in the last step. Now, for the packet to propagate forward we need $v_G > 0$, but since the denominator is negative this means $k'_x < 0$.

Then, we will have

$$r = \frac{k_x - k'_x}{k_x + k'_x} \implies \mathcal{R} = \left|\frac{k_x - k'_x}{k_x + k'_x}\right|^2 > 1\,, \tag{1.105}$$

while the other coefficient is

$$\mathcal{T} = \frac{k'_x}{k_x}|t|^2 = \frac{k'_x}{k_x}\left|\frac{2k_x}{k'_x + k_x}\right|^2 = k'_x \frac{4k_x}{(k'_x + k_x)^2} < 0\,. \tag{1.106}$$

So, we can still maintain the condition $\mathcal{R} + \mathcal{T} = 1$, but reflection is "more than certain"? Surely this is not the correct physical interpretation.

This is the heart of the Klein-Gordon paradox.

What is actually happening is that in our description we are fixing the number of particles to be one; a proper ("grand-canonical" instead of "canonical", in statistical mechanics terms) description of the situation would allow us to see that the energy in the system is enough to create real particle-antiparticle pairs.

The antiparticles gain energy under the potential (since they perceive it as $-V_0$, having a negative charge), so they are transmitted, while the particles are reflected. On average, then, more than one particle is reflected.

In order to properly study these extreme conditions, we need the new paradigm of *Quantum Field Theory*.

1.4 The Dirac Equation

Saturday 2020-3-28, compiled 2020-03-31

The Klein Gordon equation, which we discussed in the previous lectures, has two main issues:

1. It is a second order equation, since we started from the relativistic dispersion relation $E^2 = M^2 + |\vec{p}|^2$, so it admits a negative as well as a positive energy solution: $E = \pm\omega_p$.
2. The charge associated with its 4-current density J^μ is not positive definite:

$$Q = \int \mathrm{d}^3x\, J^0(\vec{x}, t) \tag{1.107}$$

can be negative.

In order to clarify the problem with these, we discussed the Klein Paradox, in which there is a violation of unitarity for a scattering process: the reflection probability was > 1 while the transmission probability was negative.

Dirac, in 1928, tried a different approach.

1.4.1 Historical derivation of the Dirac equation

We want to build an equation in the form

$$i\frac{\partial}{\partial t}\psi = H_D\psi\,, \tag{1.108}$$

for some Dirac Hamiltonian H_D, which we require to be first-order in the space derivatives and the mass, so that our equation can be covariant: this in general will be written as

$$H_D = -i\vec{\alpha}\cdot\vec{\nabla} + \beta M = \vec{\alpha}\cdot\left(-i\vec{\nabla}\right) + \beta M\,, \tag{1.109}$$

for some yet to be determined 4 coefficients $\vec{\alpha}$ and β.

Why are we introducing the i? This formulation is equivalent to saying that the energy E is given by $\vec{\alpha}\cdot\vec{p} + \beta M$, since $\vec{p} = -i\vec{\nabla}$.

We are assuming the coefficients to be constant, we shall see that this hypothesis works out. Also, as we shall these cannot be numbers, but instead they are matrices: for now, all this means is that we need to be careful when manipulating them, since in general they will not commute.

In order to determine $\vec{\alpha}$ and β we impose the conditions:

1. the Dirac Hamiltonian H_D is hermitian, since it needs to describe the physical property of energy, therefore it is an observable;

2. if ψ solves the Dirac equation, then it also solves the KG equation.

Are KG solutions also Dirac solutions generally?

The first condition can be written as $H = H^\dagger$, but to find out what it means for the coefficients $\vec{\alpha}$ and β we need to know what $\vec{\nabla}^\dagger$: since we know that momentum $\vec{p} = -i\vec{\nabla}$ is self adjoint, we must have $\vec{p}^\dagger = (-i)^\dagger\vec{\nabla}^\dagger = i\vec{\nabla}^\dagger \overset{!}{=} -i\vec{\nabla} = \vec{p}$, which means that $\vec{\nabla}^\dagger = -\vec{\nabla}$. So, we get

$$H^\dagger = (-i)^\dagger\vec{\alpha}^\dagger\cdot\vec{\nabla}^\dagger + \beta^\dagger M^\dagger \tag{1.110a}$$

$$= -i\alpha^*\cdot\vec{\nabla} + \beta^* M\,, \tag{1.110b}$$

since M is real.[5] Therefore, the coefficients must satisfy $\vec{a}^* = \vec{\alpha}$ and $\beta^* = \beta$ themselves.

The other condition, consistency with the KG equation, means that when we square the Dirac time derivative operator

$$\frac{\partial}{\partial t} = -iH_D \tag{1.111}$$

[5] In the professor's notes this is done explicitly by integrating by parts: this method can be adapted to look like that, since one can use integration by parts to show that for any wavefunctions ϕ and ψ we have $\langle\phi|\nabla\psi\rangle + \langle\nabla\phi|\psi\rangle = 0$. Then, the only difference between the approaches is whether we only integrate by parts to get the adjoint of ∇ or the whole of H_D.

we should get the KG square time- derivative operator

$$\frac{\partial^2}{\partial t^2} = \nabla^2 + M^2 \,. \tag{1.112}$$

So, we find

$$\begin{aligned}
\nabla^2 + M^2 &\stackrel{!}{=} (-iH_D)^2 = -H_D^2 && \text{(1.113a)}\\
&= -\big(-i\alpha_i\nabla_i + \beta\big)\Big(-i\alpha_j\nabla_j + \beta\Big) && \text{(1.113b)}\\
&= \alpha_i\alpha_j\nabla_i\nabla_j + i\big(\alpha_i\beta + \beta\alpha_i\big)\nabla_i + \beta^2 && \text{(1.113c)}\\
&= \frac{1}{2}\Big\{\alpha_i, \alpha_j\Big\}\nabla_i\nabla_j + i\big\{\alpha_i, \beta\big\}\nabla_i + \beta^2 \,, && \text{(1.113d)}
\end{aligned}$$

where we introduced the anticommutator bracket notation:

$$\{A, B\} = AB + BA \qquad \text{while} \qquad [A, B] = AB - BA \,. \tag{1.114}$$

So, in order for the equations to be equivalent we need to impose

$$\frac{1}{2}\Big\{\alpha_i, \alpha_j\Big\} = \delta_{ij} \qquad\qquad \big\{\alpha_i, \beta\big\} = 0 \qquad\qquad \beta^2 = M^2 \,. \tag{1.115}$$

This means α_i and β cannot be real or complex numbers: for complex numbers x, y we have $\big\{x, y\big\} = 2xy$, since for them multiplication is commutative.

Specifically, they must be matrices in an N-dimensional vector space, called a spinorial space. So, α_i and β are $N \times N$ matrices, while the wavefunction ψ is an N dimensional vector (spinor). N is yet to be determined.

They must be Hermitian matrices, since they satisfy $\alpha_i^\dagger = \alpha_i$ and $\beta^\dagger = \beta$.

We must have $\alpha_i^2 = \frac{1}{2}\{\alpha_i, \alpha_i\} = \mathbb{1}$, where $\mathbb{1}$ is the N dimensional identity matrix. Also, $\beta^2 = \mathbb{1}$. If we write α_i and β in diagonal form, which we can do since they are Hermitian, we get their real eigenvalues on the diagonal. If we square them we get the identity, therefore they must all be ± 1.

Now, let us show that these are traceless: call c_μ one of the four $\big(\beta, \alpha_i\big)$. Then, we know that $\Big\{c_\mu, c_\nu\Big\} = 2\delta_{\mu\nu}$. So, we do the following manipulation: take c_μ and c_ν, with $\nu \neq \mu$:

$$\begin{aligned}
\operatorname{Tr}\Big(c_\mu\Big) &= \operatorname{Tr}\Big(c_\mu c_\nu c_\nu\Big) && \text{(1.116a)} && c_\nu^2 = \mathbb{1}\\
&= \operatorname{Tr}\Big(-c_\nu c_\mu c_\nu\Big) && \text{(1.116b)} && \Big\{c_\mu, c_\nu\Big\} = 0, \text{ so } c_\mu c_\nu = -c_\nu c_\mu\\
&= \operatorname{Tr}\Big(-c_\mu c_\nu c_\nu\Big) && \text{(1.116c)} &&\\
&= -\operatorname{Tr}\Big(c_\mu\Big) \,, && \text{(1.116d)} && \text{Cyclic property of the trace, and linearity of the trace}
\end{aligned}$$

so $\operatorname{Tr}\Big(c_\mu\Big) = -\operatorname{Tr}\Big(c_\mu\Big) \implies \operatorname{Tr}\Big(c_\mu\Big) = 0$. Since the trace is the sum of the eigenvalues, which are ± 1, the dimension must be even.

So, our simplest guess will be $N = 2$: a basis for Hermitian complex matrices is $\{\mathbb{1}, \sigma_i\}$ where σ_i are the Pauli matrices. However, $\mathbb{1}$ is not traceless: so our c_μ can only be written as $c_\mu = \vec{c} \cdot \vec{\sigma}$.

Now, our c_μ must be linearly independent over $\mathbb{C}$: if they were not, say because $c_\mu = z c_\nu$, with $\mu \neq \nu$ and $z \in \mathbb{C}$, then the anticommutation would read

$$\left\{c_\mu, c_\nu\right\} = \{z c_\nu, c_\nu\} = z\mathbb{1} \neq 0\,, \tag{1.117}$$

a contradiction. We only have three linearly independent Pauli matrices σ_i to express four c_μ, so this cannot work.

Do however note that if $M = 0$ then we do not need the β matrix since the term multiplying it goes to zero, so the only matrices we need are the three α_i: in the massless case, then, we can use the Pauli matrices, setting $\sigma_i = \alpha_i$ satisfies all our requirements, since $\left\{\sigma_i, \sigma_j\right\} = 2\delta_{ij}$.

The next possible dimensionality is $N = 4$, and we can use the following matrices:

$$\alpha_i = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix} \qquad \text{and} \qquad \beta = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{bmatrix}. \tag{1.118a}$$

These are self adjoint since the Pauli matrices are, manifestly traceless, and they satisfy the anticommutation relations.

Proof. We expand the relation $\left\{\alpha_i, \alpha_j\right\}$: if we write $\alpha_i \alpha_j$ we get

$$\alpha_i \alpha_j = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix} \begin{bmatrix} 0 & \sigma_j \\ \sigma_j & 0 \end{bmatrix} = \begin{bmatrix} \sigma_i \sigma_j & 0 \\ 0 & \sigma_i \sigma_j \end{bmatrix}, \tag{1.119a}$$

therefore

$$\left\{\alpha_i, \alpha_j\right\} = \begin{bmatrix} \left\{\sigma_i, \sigma_j\right\} & 0 \\ 0 & \left\{\sigma_i, \sigma_j\right\} \end{bmatrix} = \left\{\sigma_i, \sigma_j\right\} \mathbb{1}_4\,, \tag{1.120a}$$

but we know that $\left\{\sigma_i, \sigma_j\right\} = 2\delta_{ij}$, so we have verified the anticommutation relations between the α_i.

To see that $\beta^2 = \mathbb{1}_4$ is immediate since it is already diagonal, so we only need to show $\left\{\alpha_i, \beta\right\} = 0$. We have

$$\alpha_i \beta = \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix} \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{bmatrix} = \begin{bmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{bmatrix} \tag{1.121a}$$

$$\beta \alpha_i = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{bmatrix} \begin{bmatrix} 0 & \sigma_i \\ \sigma_i & 0 \end{bmatrix} = \begin{bmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{bmatrix}, \tag{1.121b}$$

so the sum $\alpha_i \beta + \beta \alpha_i$ is zero, which proves our statement. □

The γ matrices

It is then conventional to define the matrices

$$\gamma^0 = \beta = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & -\mathbb{1} \end{bmatrix} \qquad \text{and} \qquad \gamma^i = \beta\alpha_i = \begin{bmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{bmatrix}, \tag{1.122a}$$

which obey the following properties:

1. $\gamma^0 = (\gamma^0)^\dagger$, while $\gamma^i = -(\gamma^i)^\dagger$;
2. $\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}$, specifically $(\gamma^0)^2 = \mathbb{1}_4$ and $(\gamma^i)^2 = -\mathbb{1}_4$.

We can then interpret this collection of matrices as a 4-vector. We can rewrite the Dirac equation using them: we multiply it by β to get

$$i\partial_0\psi = \left(-i\alpha_i\partial_i + \beta M\right)\psi \tag{1.123a}$$

$$i\beta\partial_0\psi = \left(-i\beta\alpha_i\partial_i + \beta^2 M\right)\psi \tag{1.123b}$$

$$i\gamma^0\partial_0\psi = \left(-\gamma^i\partial_i + \beta^2 M\right)\psi \tag{1.123c}$$

$$\left(i\gamma^\mu\partial_\mu - M\right)\psi = 0\,. \tag{1.123d}$$

This looks simple, but recall that γ^μ are 4×4 matrices and ψ is a 4D spinor: if we write this explicitly using the spinor indices, for which we use the Hebrew letters א nd ב (aleph and beth[6]), we get

$$\left(i\gamma^\mu_{\aleph\beth} - M\delta_{\aleph\beth}\right)\psi_\beth = 0\,, \tag{1.124}$$

which is a set of 4 equations, indexed by the free index א. Since the γ matrices are not diagonal, the components $\psi_\beth$ are mixed in the equation.

If we introduce the slashed notation $\not{p} \stackrel{\text{def}}{=} \gamma^\mu p_\mu$.

With this notation, the Dirac equation reads

$$\boxed{\left(i\not{\partial} - M\right)\psi = 0\,.} \tag{1.125}$$

Representations of γ-matrices

The way we defined the γ matrices was arbitrary, and in fact there are other possible equivalent definitions which are also physically useful.

In general, for any unitary matrix C we can move to the new representation

$$\widetilde{\gamma}^\mu = C^{-1}\gamma^\mu C\,. \tag{1.126}$$

[6] Since this notation will only be used here, it does not matter if it is a little inconvenient. I did not use greek or latin letters since they both already have meaning in the conventional notation.

How do we prove that the physical results are the same? The Dirac equation is in the form $A\psi = 0$, and if we show that for an equation in this form $C^{-1}AC$ is as good as A then we are done: in $A = i\partial\!\!\!/ - M\mathbb{1}$ the $M\mathbb{1}$ term is unaffected since it commutes with the matrix, the derivative is unaffected since the C matrix is assumed to be constant. But then, if we want to use $\widetilde{A} = C^{-1}AC$, we will find solutions to $C^{-1}ACC^{-1}\psi = \widetilde{A}\widetilde{\psi}$, where $\widetilde{\psi} = C^{-1}\psi$: we do not lose any information, sure, since the matrix is unitary, but is the state physically equivalent?

The Dirac representation we gave before is usually used when dealing with the non-relativistic limit, while the one we now show is called the relativistic, or Weyl, or chiral, representation. We use the matrix which is known in quantum information as the Hadamard gate:

$$C = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \tag{1.127a}$$

we can move to the representation

$$\gamma^\mu = \left(\begin{bmatrix} 0 & \mathbb{1} \\ \mathbb{1} & 0 \end{bmatrix}, \begin{bmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{bmatrix} \right). \tag{1.128a}$$

Proof. We multiply, writing 1 for $\mathbb{1}$ and 0 for the 0 matrix for simplicity: for γ^0 we get

$$C^{-1}\gamma^0 C = \frac{1}{2} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \tag{1.129a}$$

$$= \frac{1}{2} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \tag{1.129b}$$

$$= \frac{1}{2} \begin{bmatrix} 0 & 2 \\ 2 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \tag{1.129c}$$

while for γ^i we have

$$C^{-1}\gamma^i C = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{bmatrix} \begin{bmatrix} 1 & -1 \\ 1 & 1 \end{bmatrix} \tag{1.130a}$$

$$= \frac{1}{2} \begin{bmatrix} 1 & 1 \\ -1 & 1 \end{bmatrix} \begin{bmatrix} \sigma_i & \sigma_i \\ -\sigma_i & \sigma_i \end{bmatrix} \tag{1.130b}$$

$$= \begin{bmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{bmatrix}. \tag{1.130c}$$

□

The Dirac equation is consistent with the Klein Gordon equation: we can multiply it by the conjugate of the Dirac operator, $-(i\not{\partial} + M)$, to get

$$-\left(i\not{\partial} + M\right)\left(i\not{\partial} - M\right)\psi = 0 \tag{1.131a}$$

$$\left(\gamma^\mu\gamma^\nu\partial_\mu\partial_\nu + M^2\right) = 0 \tag{1.131b}$$

$$\left(\Box + M^2\right)\psi = 0\,, \tag{1.131c}$$

which is equivalent to the Klein-Gordon equation since when we compute $\gamma^\mu\gamma^\nu\partial_\mu\partial_\nu$ we only have the symmetric part, since the partial derivatives commute, and $\frac{1}{2}\{\gamma^\mu, \gamma^\nu\} = \eta^{\mu\nu}$.

The Klein-Gordon equation is then diagonal in the spinorial space: by this manipulation we have shown that the KG operator is proportional to the identity.

1.4.2 Covariance of the Dirac Equation

Sunday 2020-3-29, compiled 2020-03-31

How do these new spinors transform under Lorentz transformations?

We suppose that for a general Lorentz transformation Λ we will have something in the form

$$\psi'(x') = S(\Lambda)\psi(x)\,, \tag{1.132}$$

where $S(\Lambda)$ is a 4×4 matrix, belonging to the *spinorial representation of the Lorentz group*. We do this because if we were to simply impose $\psi'(x') = \psi(x)$ we get a contradiction, so the equation is not covariant.

Now, let us see what we must require of the matrices $S(\Lambda)$ so that the Dirac equation holds in the new frame as well as in the old. When we do the computation, recall that the γ^μ matrices are *not* a 4-vector, despite the position of the index: they need not be transformed using a Λ matrix; better put, they are a set of 4 Lorentz scalars

So, we must have

$$\left(i\not{\partial}' - M\right)\psi'(x') = \left(i\gamma^\mu\Lambda_\mu{}^\nu\partial_\nu - M\right)S(\Lambda)\psi(x) \tag{1.133a}$$

$$= S(\Lambda)\left[i\Lambda_\mu{}^\nu S^{-1}(\Lambda)\gamma^\mu S(\Lambda)\partial_\nu - M\right]\psi(x) \tag{1.133b}$$

$$= S(\Lambda)\left[i\not{\partial} - M\right]\psi(x)\,, \tag{1.133c}$$

where we used the following:

1. the matrix $S(\Lambda)$ is constant with respect to the spatial coordinates, since the Lorentz transformation is fixed, so we can bring it outside of the derivative ∂_ν;
2. the matrices γ^μ and $S(\Lambda)$ do not commute *a priori*, so if we wish to bring the equation in the form $S(\Lambda)\times\left[\text{old-coordinates Dirac eq}\right]$ we cannot simply commute them, instead we multiply by $\mathbb{1} = SS^{-1}$ on the left;
3. we impose the condition

$$\Lambda_\mu{}^\nu S^{-1}(\Lambda)\gamma^\mu S(\Lambda) \overset{!}{=} \gamma^\nu \tag{1.134}$$

in order to find the expression we need in order for the equation to be covariant, since as long as the matrix $S(\Lambda)$ is nondegenerate the equation $S(\Lambda)\left[i\partial\!\!\!/ - M\right]\psi = 0$ has the same solutions as the Dirac equation.

If we multiply by an inverse Lorentz matrix on both sides we can bring this equation into the form

$$S^{-1}(\Lambda)\gamma^\mu S(\Lambda) = \Lambda^\mu{}_\nu \gamma^\nu \,, \tag{1.135}$$

so we can say that the Dirac equation is covariant as long as we find some matrices $S(\Lambda)$ satisfying these conditions. Do note that while this looks like a vector transformation law, the γ^μ matrices do not transform under Lorentz transformations: what we are stating is that it is equivalent to apply a Lorentz matrix to them and to transform them as spinorial matrices.

In a way, we are asking the transformation laws for spinors and vectors to be compatible.

Explicit realization of the spinorial representation

In order to do this, we consider infinitesimal Lorentz transformations,

$$\Lambda^\mu{}_\nu = \delta^\mu{}_\nu + \omega^\mu{}_\nu \,, \tag{1.136}$$

where $\omega_{\mu\nu} = \omega_{[\mu\nu]}$ is an antisymmetric tensor.[7]

A rank-2 antisymmetric tensor in 4 dimensions has 6 degrees of freedom: these physically correspond to three rotations and three boosts.

A rather general ansatz looks like:

$$S(\Lambda) = \mathbb{1} - \frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu} \,, \tag{1.137}$$

where $\Sigma^{\mu\nu}$ is the set of the generators of the spinorial representation of the Lorentz group. For fixed μ and ν, these are matrices in the spinor space: if we write all the indices explicitly, they look like $\Sigma^{\mu\nu}_{\aleph\beth}$.

This means that to each possible basis Lorentz transformation of spacetime (think boost or rotation) we are associating a 4×4 basis spinor transformation matrix. This is what finding a representation of the group means: for each element of the Lorentz group we are finding a transformation matrix.

Do note, however, that we are only working at linear order in $\omega_{\mu\nu}$, so we are not looking yet at a representation of the whole group, instead we are only considering elements which are close to the identity. So, we can insert this expression for $S(\Lambda)$ into the relation between the $S(\Lambda)$ and Λ, equation (1.135), using the fact that to first order $S = \mathbb{1} + \epsilon$ is the inverse of $S^{-1} = \mathbb{1} - \epsilon$ we have, to first order in ω:

$$\left(\mathbb{1} + \frac{i}{2}\omega_{\rho\sigma}\Sigma^{\rho\sigma}\right)\gamma^\mu\left(\mathbb{1} - \frac{i}{2}\omega_{\alpha\beta}\Sigma^{\alpha\beta}\right) = \gamma^\mu + \omega^\mu{}_\nu\gamma^\nu \tag{1.138a}$$

[7] The fact that ω must be antisymmetric may be derived by imposing the condition $\eta_{\mu\nu} = \Lambda_\mu{}^\alpha \Lambda_\nu{}^\beta \eta_{\alpha\beta}$, with the perturbed Λ we wrote above.

$$\gamma^\mu + \frac{i}{2}\omega_{\rho\sigma}\Sigma^{\rho\sigma}\gamma^\mu - \frac{i}{2}\gamma^\mu\omega_{\alpha\beta}\Sigma^{\alpha\beta} = \gamma^\mu + \omega_{\sigma\nu}\eta^{\mu\sigma}\gamma^\nu \tag{1.138b}$$

$$-\frac{i}{2}\omega_{\rho\sigma}\left[\gamma^\mu, \Sigma^{\rho\sigma}\right] = \omega_{\sigma\nu}\eta^{\mu[\sigma}\gamma^{\nu]} \tag{1.138c}$$

$$\left[\gamma^\mu, \Sigma^{\rho\sigma}\right] = i\left(\eta^{\mu\rho}\gamma^\sigma - \eta^{\mu\sigma}\gamma^\rho\right), \tag{1.138d}$$

where we antisymmetrized the indices in $\eta^{\mu\rho}\gamma^\sigma$ since they are multiplied by the antisymmetric tensor $\omega_{\rho\sigma}$, so any symmetric part would not contribute to the equation. We also used the fact that $\omega_{\rho\sigma}$ is proportional to the identity in the spinor space.

Claim 1.4.1. *This is satisfied by*

$$\Sigma^{\mu\nu} = \frac{i}{4}[\gamma^\mu, \gamma^\nu] = \frac{1}{2}\sigma^{\mu\nu}, \tag{1.139}$$

Proof. We plug the definitions in:

$$\left[\gamma^\mu, \Sigma^{\rho\sigma}\right] = \frac{i}{4}\left(\gamma^\mu\gamma^\rho\gamma^\sigma - \gamma^\mu\gamma^\sigma\gamma^\rho - \gamma^\rho\gamma^\sigma\gamma^\mu + \gamma^\sigma\gamma^\rho\gamma^\mu\right) \tag{1.140a}$$

$$i\left(\eta^{\mu\rho}\gamma^\sigma - \eta^{\mu\sigma}\gamma^\rho\right) = \frac{i}{2}\left(\gamma^\mu\gamma^\rho\gamma^\sigma + \gamma^\rho\gamma^\mu\gamma^\sigma - \gamma^\mu\gamma^\sigma\gamma^\rho - \gamma^\sigma\gamma^\mu\gamma^\rho\right), \tag{1.140b}$$

where we used the anticommutation relations $\{\gamma^\mu, \gamma^\nu\} = 2\eta^{\mu\nu}$. Then, we must check whether these two expression are equal, that is, whether

$$\frac{1}{2}\left(\mu\rho\sigma - \mu\sigma\rho - \rho\sigma\mu + \sigma\rho\mu\right) \stackrel{?}{=} \mu\rho\sigma + \rho\mu\sigma - \mu\sigma\rho - \sigma\mu\rho \tag{1.141a}$$

$$= \{\mu, \rho\}\sigma - \{\mu, \sigma\}\rho, \tag{1.141b}$$

where we only write the indices of the γs for clarity.

We can now use the identity:

$$[\mu, \rho\sigma] = \mu\rho\sigma - \rho\sigma\mu \tag{1.142a}$$

$$= \mu\rho\sigma + \rho\mu\sigma - \rho\mu\sigma - \rho\sigma\mu \tag{1.142b}$$

Added and subtracted

$$= \{\mu, \rho\}\sigma - \rho\{\mu, \sigma\}. \tag{1.142c}$$

Note that in our convention there is no division by 2 in the commutator and anticommutator. Then, we can recognize these in the initial claim: we find

$$\frac{1}{2}\left(\mu\rho\sigma - \mu\sigma\rho - \rho\sigma\mu + \sigma\rho\mu\right) = \frac{1}{2}\Big(\left[\mu, \rho\sigma\right] - \left[\mu, \sigma\rho\right]\Big) \tag{1.143a}$$

$$= \frac{1}{2}\Big(\{\mu, \rho\}\sigma - \rho\{\mu, \sigma\} - \{\mu, \sigma\}\rho + \sigma\{\mu, \rho\}\Big) \tag{1.143b}$$

$$= \{\mu, \rho\}\sigma - \{\mu, \sigma\}\rho, \tag{1.143c}$$

since the anticommutators $\{\mu, \sigma\}$ are proportional to the metric $\eta^{\mu\sigma}$, which is proportional to the identity in the spinorial space, which commutes with the gamma matrices, so $\{\mu, \sigma\}$ commutes with any gamma matrix. □

Up until now we have worked "near the identity" of our transformation group; if we want to extrapolate these results to general transformations we may use the exponential map, which gives us relations in the form

$$S(\Lambda) = \exp\left(-\frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu}\right) \tag{1.144a}$$

$$S^{-1}(\Lambda) = \exp\left(\frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu}\right). \tag{1.144b}$$

1.4.3 Dirac conjugate spinor

We want to define a notion of a conjugate spinor, starting from what we know about hermitian conjugate operators: we start by taking the Hermitian conjugate of the Dirac equation,

$$\left[\left(i\partial\!\!\!/ - M\right)\psi\right]^\dagger = -i\psi^\dagger\left(i\gamma^{\mu\dagger}\overleftarrow{\partial}_\mu + M\right), \tag{1.145}$$

where the result follows from the fact that the adjoint of a product is the product of the reverse-ordered adjoints, while the notation $\overleftarrow{\partial}_\mu$ means that the derivative operator is acting on what is on its left.

In order to simplify this, we employ the following facts: $(\gamma^0)^2 = \mathbb{1}$, and

$$\gamma^0\gamma^{\mu\dagger}\gamma^0 = \gamma^\mu. \tag{1.146}$$

Proof. For γ^0 the result is immediate, since it is self adjoint: $\gamma^0 = \gamma^{0,\dagger}$, so the expression reduces to $\left(\gamma^0\right)^3 = \left(\gamma^0\right)^2\left(\gamma^0\right) = \gamma^0$.

Then let us consider γ^i: since they are block matrices of the Pauli matrices, which are self-adjoint and which have determinant -1, we have:

$$\gamma^{i\dagger} = \begin{bmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{bmatrix}^\dagger = \begin{bmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{bmatrix} = -\gamma^i, \tag{1.147a}$$

therefore we need to prove that $\gamma^0\gamma^i\gamma^0 = -\gamma^i$:

$$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & \sigma_i \\ -\sigma_i & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}\begin{bmatrix} 0 & -\sigma_i \\ -\sigma_i & 0 \end{bmatrix} \tag{1.148a}$$

$$= \begin{bmatrix} 0 & -\sigma_i \\ \sigma_i & 0 \end{bmatrix}. \tag{1.148b}$$

□

With these results, we can use the manipulation

$$\psi^\dagger\gamma^{\mu\dagger}\overleftarrow{\partial}_\mu = \psi^\dagger\gamma^0\gamma^0\gamma^{\mu\dagger}\gamma^0\gamma^0\overleftarrow{\partial}_\mu \tag{1.149a}$$

$$= \psi^\dagger \gamma^0 \gamma^\mu \overleftarrow{\partial}_\mu \gamma^0 \,, \tag{1.149b}$$

which holds since the matrix γ^0 is constant. We also define $\overline{\psi} = \psi^\dagger \gamma^0$, so that the whole equation reads

$$\overline{\psi}(i\partial\!\!\!/ + M) = 0 \,, \tag{1.150}$$

where we removed the γ^0 at the right, since the equation multiplied by it is equivalent to the one which is not.

Now, in order to see how $\overline{\psi}$ transforms under a Lorentz transformation we use the following facts:

1. $\psi'(x') = S(\Lambda)\psi(x)$ and
2. $\gamma^0 S^\dagger(\Lambda)\gamma^0 = S^{-1}(\Lambda)$.

Proof. We are going to work near the identity: this is justified, since if we find an equality like $f(\Lambda) \equiv g(\Lambda)$ for Λ near $\mathbb{1}$, then we can extrapolate it using the exponential map to places further away in the group.

Does this actually work, or are we deriving something which only holds near the identity?

We know that $S(\Lambda)$ is written as

$$S(\Lambda) = \exp\left(-\frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu}\right) , \tag{1.151}$$

so its adjunct is

$$S^\dagger(\Lambda) = \exp\left(\frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu\dagger}\right) \approx \mathbb{1} + \frac{i}{2}\omega_{\mu\nu}\Sigma^{\mu\nu\dagger} \,, \tag{1.152}$$

so when we multiply it from the left and right by γ^0 it goes through everything, and we are left with

$$\gamma^0 \Sigma^{\mu\nu\dagger} \gamma^0 \stackrel{?}{=} \Sigma^{\mu\nu} \,, \tag{1.153}$$

since the expression for $S^{-1}(\Lambda)$ differs from that of $S(\Lambda)$ only for a sign in the exponent, but we picked up a sign when taking the adjunct. Recall that the explicit expression of the Σ matrices is

$$\Sigma^{\mu\nu} = \frac{i}{4}[\gamma^\mu, \gamma^\nu] \,, \tag{1.154}$$

so we can show directly that

$$\gamma^0 \Sigma^{\mu\nu\dagger} \gamma^0 = \frac{i}{4}\gamma^0\gamma^{\mu\dagger}\gamma^{\nu\dagger}\gamma^0 - \frac{i}{4}\gamma^0\gamma^{\nu\dagger}\gamma^{\mu\dagger}\gamma^0 \tag{1.155a}$$

$$= \frac{i}{4}\gamma^0\gamma^{\mu\dagger}\gamma^0\gamma^0\gamma^{\nu\dagger}\gamma^0 - \frac{i}{4}\gamma^0\gamma^{\nu\dagger}\gamma^0\gamma^0\gamma^{\mu\dagger}\gamma^0 \tag{1.155b}$$

$$= \frac{i}{4}[\gamma^\mu\gamma^\nu] = \Sigma^{\mu\nu} \,. \tag{1.155c}$$

□

Using these results, we can show that the conjugate spinor $\overline{\psi} = \psi^\dagger \gamma^0$ transforms like:

$$\begin{aligned}
\overline{\psi}'(x') &= \psi'^\dagger \gamma^0 && \text{(1.156a)}\\
&= \big(S(\Lambda)\psi\big)^\dagger \gamma^0 && \text{(1.156b)}\\
&= \psi^\dagger S^\dagger(\Lambda)\gamma^0 && \text{(1.156c)}\\
&= \psi^\dagger \gamma^0\gamma^0 S^\dagger(\Lambda)\gamma^0 && \text{(1.156d)}\\
&= \overline{\psi} S^{-1}(\Lambda) && \text{(1.156e)}\\
&. && \text{(1.156f)}
\end{aligned}$$

1.4.4 Continuity equation

We can apply the same strategy we used in the KG case: if we multiply the Dirac equation by $\overline{\psi}$ on the left and the conjugate equation by ψ on the right, we get

$$\overline{\psi}(i\partial\!\!\!/ - M)\psi = 0 \overline{\psi}\left(i\overleftarrow{\partial\!\!\!/} + M\right)\psi \qquad = 0\,. \tag{1.157}$$

if we sum them, the $M\overline{\psi}\psi$ terms cancel, so we have

$$\begin{aligned}
0 &= \overline{\psi}\left(i\overleftarrow{\partial\!\!\!/} + i\partial\!\!\!/\right)\psi && \text{(1.158a)}\\
&= i\Big((\partial_\mu\overline{\psi})\gamma^\mu\psi + \overline{\psi}\gamma^\mu\partial_\mu\psi\Big) && \text{(1.158b)}\\
&= \partial_\mu\big(\overline{\psi}\gamma^\mu\psi\big)\,, && \text{(1.158c)}
\end{aligned}$$

so we have the conserved current $\overline{\psi}\gamma^\mu\psi = J^\mu$. Its corresponding charge density is $\rho = J^0 = \overline{\Psi}\gamma^0\psi = \psi^\dagger\psi$.

This looks like a positive definite conserved charge, so it could be interpreted as a probability. In fact, this is not the case, as we shall see in the future.

1.4.5 Bilinear forms and Lorentz transformations

Our observables can not still carry spinorial indices: all the spinorial indices must be saturated in the expression for an observable, since we can only observe scalars in the spin tensor algebra.

For instance, $\overline{\psi}\psi$ is the dot product of two spinors, so it carries no indices. It is a scalar under Lorentz transformations, since $\overline{\psi}$ transforms with a S^{-1} while ψ transforms with an S.

$\overline{\psi}\gamma^\mu\psi$ is instead a vector under Lorentz transformations: it transforms like

$$\overline{\psi}\gamma^\mu\psi \to \overline{\psi}S^{-1}(\Lambda)\gamma^\mu S(\Lambda)\psi = \overline{\psi}\Lambda^\mu{}_\nu\gamma^\nu\psi\,, \tag{1.159}$$

where we used the property shown in equation (1.135).

So, everything we are doing is covariant when we are discussing observables.

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