Lecture Notes

Wave Equations of Relativistic Quantum Mechanics

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1. Background

In this course, we will discuss relativistic quantum mechanical wave equations such as the Klein-Gordon equation

$$\left(\frac{1}{c^2}\frac{\partial}{\partial t^2} - \Delta + \frac{m^2c^2}{\hbar^2}\right)\psi(t,\mathbf{x}) = 0 \tag{1.1}$$

and the Dirac equation

$$\sum_{\mu=0}^{3} i\hbar\gamma^\mu \frac{\partial\psi}{\partial x^\mu} - mc\,\psi = 0, \tag{1.2}$$

where $\gamma^\mu,\ \mu = 0,1,2,3$ are certain 4×4 matrices.

The basic motivation is that the Schrödinger equation

$$i\hbar\partial_t\psi(t,\mathbf{q}) = \left(-\frac{\hbar^2}{2m}\Delta + V(t,\mathbf{q})\right)\psi(t,\mathbf{q}) \tag{1.3}$$

is not invariant under the basic symmetry transformations of (special) relativity, Lorentz transformations. There are two reasons for this:

1. The Schrödinger equation contains just a first order time derivative but second order spatial derivatives. As Lorentz transformations mix spatial and time derivatives, it cannot be Lorentz invariant.

2. For many ($N \in \mathbb{N}$) particles, $q = (\mathbf{x}_1, ..., \mathbf{x}_N)$. Then the object $\psi(t, \mathbf{x}_1, ..., \mathbf{x}_N)$ contains one time variable and N space variables, hence it is unclear how to Lorentz transform it. (We would need N *spacetime* variables for that.)

We shall address both points. For a single particle, reason 1 will lead us to the Klein-Gordon and the Dirac equations. Reason 2 will come into play later when we consider many particles in the multi-time formalism of Dirac, Tomonaga and Schwinger. (The central idea is to consider multi-time wave functions $\psi(x_1, ..., x_N)$ with one spacetime argument x_i for each particle.)

The relativistic wave equations have several interesting and new features. Both Klein-Gordon and Dirac equations admit negative energies. These have to do with antiparticles, and indeed the Dirac equation has historically led to the concept of the positron. The Dirac equation automatically includes spin, and thus gives a reason why (fermionic) particles should have spin.

In elementary particle physics, especially the Dirac equation is of fundamental importance and occurs at a central place in the Standard Model. It is used to describe all the elementary fermions. The Klein-Gordon equation is often used as a

toy model, and even more seriously for the description of spin-0 bosons such as the Higgs particle.

Both the Klein-Gordon equation and the Dirac equation are important examples for hyperbolic partial differential equations. 'Hyperbolic' means that the equation distinguishes one special direction that plays the role of time. The two equations also have a canonical generalization to curved spacetimes as in general relativity (we will not do this here, though). Moreover, the Dirac equation leads to non-trivial representations of the Lorentz group, so called *spinor representations*. This has led to a whole area of research in theoretical and mathematical physics. In pure mathematics, the Dirac operator also plays an important role in differential geometry and index theory.

1.1 Basics of non-relativistic quantum mechanics

Wave function. Our discussion takes place in the Schrödinger picture of QM. The basic object of QM then is a time-dependent wave function

$$\psi : \mathbb{R} \times \underbrace{\mathbb{R}^3 \times \cdots \times \mathbb{R}^3}_{N} \to \mathbb{C}^k, \quad (t, \underbrace{\mathbf{x}_1, ..., \mathbf{x}_N}_{\mathbf{q}}) \mapsto \psi(t, \mathbf{x}_1, ..., \mathbf{x}_N). \tag{1.4}$$

Here, N is the number of particles described (in a rather indirect way) by ψ. k is the number of components of ψ. It depends on the type of the particle. The most important examples are spin-0 ($k = 0$) and spin-$\frac{1}{2}$ particles ($k = 2^N$).

Schrödinger equation. The governing equation of QM reads (setting $\hbar = 1$):

$$i\partial_t \psi(t, \mathbf{q}) = \left(-\frac{1}{2m} \Delta_q + V(t, \mathbf{q}) \right) \psi(t, \mathbf{q}). \tag{1.5}$$

Here, Δ_q is the Laplacian on the configuration space $\mathbb{R}^{3N}$ and $V(t, \mathbf{q})$ a potential. m stands for the mass of the particles (they are assumed to have the same mass here).

Invariance under Galilean transformations. Galilean transformations are the symmetry transformations of non-relativistic spacetime. They describe the change of coordinates from one inertial frame F to another F' which moves with uniform velocity $-\mathbf{u}$ with respect to the other. The coordinates in F are denoted by $(t, \mathbf{x}) \in \mathbb{R}^4$ and in F' by $(t', \mathbf{x}') \in \mathbb{R}^4$ They are combinations of the following elementary transformations:

1. *Space and time translations.* For $\tau \in \mathbb{R}$ and $\mathbf{a} \in \mathbb{R}^3$: $t' = t + \tau$, $\mathbf{x}' = \mathbf{x} + \mathbf{a}$.
2. *Rotations.* For a rotation matrix $R \in O(3)$: $t' = t$, $\mathbf{x}' = R\mathbf{x}$.
3. *Galilean boosts.* For a velocity $\mathbf{u} \in \mathbb{R}^3$: $t' = t$, $\mathbf{x}' = \mathbf{x} + \mathbf{u}t$.

These transformations were for $\mathbf{x} \in \mathbb{R}^3$ (physical space). For configuration space, one transforms each $\mathbf{x}_i$ in $\mathbf{q} = (\mathbf{x}_1, ..., \mathbf{x}_N)$ in the same manner.

Now, what does "Galilean invariance" of the Schrödinger equation mean? It means that we specify a rule how to calculate a transformed $\psi'(t', \mathbf{x}')$ that refers

to the new frame F' from the previous $\psi(t, \mathbf{x})$ for F. This rule must be such that if $\psi(t, \mathbf{x})$ solves the Schrödinger equation w.r.t. $(t, \mathbf{x})$, then $\psi'(t', \mathbf{x}')$ solves the Schrödinger equation w.r.t. $(t', \mathbf{x}')$.

We focus on the case of $N = 1$ particles and set $V = 0$ (for $N > 1$, the only requirement for V is that it is a Galilean invariant function, such as the Coulomb potential). For the Schödinger equation, the transformation rules for the Galilean transformations 1-3 are:

1. $\psi'(t', \mathbf{x}') = \psi(t, \mathbf{x}) = \psi(t' - \tau, \mathbf{x}' - \mathbf{a})$,
2. $\psi'(t', \mathbf{x}') = \psi(t, \mathbf{x}) = \psi(t', R^T \mathbf{x}')$,
3. Here a novel feature appears: The transformation $\psi'(t', \mathbf{x}') = \psi(t, \mathbf{x}) = \psi(t', \mathbf{x}' - \mathbf{u}t')$ does not lead to invariance. One needs to include a factor Φ depending on $(t', \mathbf{x}', \mathbf{u})$:
$$\psi'(t', \mathbf{x}') = \Phi(t', \mathbf{x}', \mathbf{u})\, \psi(t', R^T \mathbf{x}') \tag{1.6}$$
The lesson is that implementing symmetry transformations on abstract spaces such as the space of wave functions can be more subtle than one may think. We will encounter this situation especially for the Dirac equation. There we will study representations of the Lorentz group more systematically.

You will demonstrate the Galilean invariance of the Schrödinger equation on **Sheet 1, Exercise 2.**

Continuity equation and Born rule. As a consequence of the Schrödinger equation, the density
$$\rho(t, \mathbf{q}) = |\psi|^2(t, \mathbf{q}) \tag{1.7}$$
and the current
$$\mathbf{j} = \frac{1}{m} \mathrm{Im}\, \psi^\dagger(t, \mathbf{q}) \nabla_q \psi(t, \mathbf{q}) \tag{1.8}$$
satisfy the *continuity equation*
$$\partial_t \rho(t, \mathbf{q}) + \mathrm{div}\, \mathbf{j}(t, \mathbf{q}) = 0. \tag{1.9}$$
You will show this on **Sheet 1, Exercise 1**.
A continuity equation describes a substance (with density ρ) which can be neither created nor destroyed but is rather just redistributed according to the current $\mathbf{j}$.

Here the conserved quantity is the *total probability* to find the particles somewhere in space,
$$P(t) = \int d^3\mathbf{x}\, |\psi|(t, \mathbf{q}). \tag{1.10}$$
The fact that $\frac{d}{dt} P(t) = 0$ follows from (1.9). However, (1.9) is stronger than this, as it means that probability is even conserved *locally*. This fact is the basis of the statistical meaning of ψ, as given by the *Born rule*:

> $|\psi|^2(t, \mathbf{x}_1, ..., \mathbf{x}_N)$ is the probability density to find, at time t, N particles at locations $\mathbf{x}_1$,...,$\mathbf{x}_N$, respectively.

This rule is crucial as it relates the abstract wave function with concrete physical predictions for particles.

Hilbert space picture. One can also regard the Schrödinger equation more abstractly as an equation on the Hilbert space

$$\mathscr{H} = L^2(\mathbb{R}^{3N}, \mathbb{C}^k) \tag{1.11}$$

of square integrable functions $\varphi : \mathbb{R}^{3N} \to \mathbb{C}^k$ with scalar product

$$\langle \varphi, \phi \rangle = \int d^3\mathbf{x}\, \varphi^\dagger(\mathbf{x})\phi(\mathbf{x}). \tag{1.12}$$

Then the Schrödinger equation takes the form

$$i\frac{d\psi(t)}{dt} = \widehat{H}\psi(t), \tag{1.13}$$

where ψ is viewed as a map $\psi : \mathbb{R} \to \mathscr{H}$ and

$$\widehat{H} = -\frac{1}{2m}\Delta + V \tag{1.14}$$

defines the Hamiltonian. One usually requires that $\widehat{H}$ is self-ajoint. Then it generates a unitary group, given by

$$U(t) = e^{-i\widehat{H}t}. \tag{1.15}$$

This unitary group yields the solution $\psi(t)$ of the initial value problem $\psi(0) = \psi_0$ of (1.13) by

$$\psi(t) = e^{-i\widehat{H}t}\,\psi_0. \tag{1.16}$$

Particular self-adjoint operators on $\mathscr{H}$ ("observables") summarize the statistics of experiments in a convenient way. Their eigenvalues correspond to the possible outcomes of the experiment, and the norms of the corresponding eigenfunctions give the probabilities with which these outcomes occur. For example, the eigenvalues of $\widehat{H}$ correspond to the values the total energy of the system can take.

Quantization recipe. One can guess the Schrödinger equation for $N = 1$ as follows. The energy momentum relation for a single particle in classical mechanics reads:

$$E = \frac{\mathbf{p}^2}{2m} + V(t, \mathbf{x}). \tag{1.17}$$

The quantization recipe now is to

(a) Exchange E and $\mathbf{p}$ with operators:

$$E \to i\hbar\partial_t, \quad \mathbf{p} \to -i\hbar\nabla. \tag{1.18}$$

V becomes a multiplication operator.

(b) Insert the operators into the energy-momentum relation and let the result act on ψ:

$$E\psi = \left(\frac{\mathbf{p}^2}{2m} + V(t, \mathbf{x})\right)\psi \quad \to \quad i\hbar\partial_t\psi = \left(-\frac{\hbar^2}{2m}\nabla^2 + V(t, \mathbf{x})\right)\psi. \tag{1.19}$$

This indeed gives the (free) Schrödinger equation. This procedure is sometimes useful for guessing quantum mechanical equations; one should not overestimate its conceptual value, though.

1.2 Basics of special relativity

Minkowski spacetime. Minkowski spacetime is the spacetime manifold of special relativity (without gravitation)[1]. It is given by $\mathbb{M} = (\mathbb{R}^4, \eta)$, i.e. four-dimensional space $\mathbb{R}^4$ equipped with the Minkowski (pseudo-) metric

$$\eta : \mathbb{M} \otimes \mathbb{M} \to \mathbb{R}, \quad (x, y) \mapsto x^T \operatorname{diag}(1, -1, -1, -1)\, y. \tag{1.20}$$

Given two points $x = (x^0, \mathbf{x})$ and $y = (y^0, \mathbf{y}) \in \mathbb{M}$, the quantity $\eta(x, y)$

$$s^2(x, y) = \eta(x - y, x - y) = (x^0 - y^0)^2 - |\mathbf{x} - \mathbf{y}|^2. \tag{1.21}$$

is called the *spacetime distance* of x and y. For equal times, we obtain (minus) the usual spatial distance squared. One distinguishes three cases:

1. $s^2(x, y) < 0$: *space-like related*. That means, x and y are "somewhere else in space" with respect to each other.

2. $s^2(x, y) > 0$: *time-like related*. That means, x is in the future of y (if $x^0 > y^0$) or x is in the past of y (if $x^0 < y^0$).

3. $s^2(x, y) = 0$: *light-like related*. That means, x and y can be connected with a light ray.

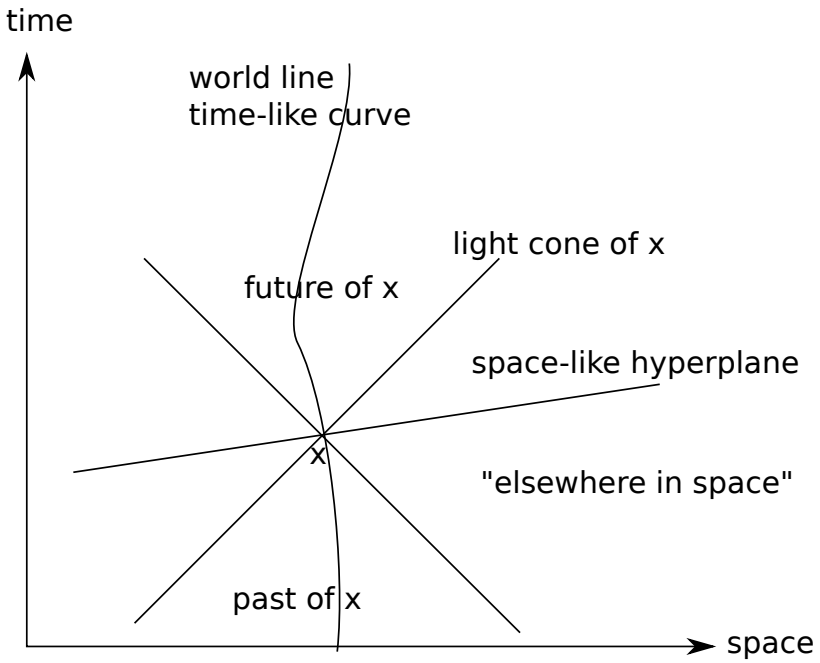

Figure 1.1: Spacetime diagram

[1]Note for experts: As Minkowski spacetime is flat as a manifold (not curved), it is also a vector space. Furthermore, all tangent spaces are isomorphic to Minkowski spacetime itself. This allows to identify these spaces with Minkowski spacetime. We shall do this in the following.

Index notation. We set $\hbar = c = 1$.
We denote *vectors* $x \in \mathbb{M}$ by $x = (x^0, x^1, x^2, x^3)$. x^μ, $\mu = 0, 1, 2, 3$ are the components of x in a particular inertial frame. The component $x^0 = ct$ corresponds to time, and the spatial components are often indicated by using roman indices x^j, $j = 1, 2, 3$. We sometimes write $x = (t, \mathbf{x})$ with $\mathbf{x} \in \mathbb{R}^3$.
Covectors $\omega \in \mathbb{M}^*$ are maps $\omega : \mathbb{M} \to \mathbb{R}$. We denote them using lower indices

$$\omega = (\omega_\mu)_{\mu=0,1,2,3}. \tag{1.22}$$

Their action on a vector x is given by

$$\omega\, x = \sum_{\mu=0}^{3} \omega_\mu x^\mu. \tag{1.23}$$

We also abbreviate this by

$$\omega_\mu x^\mu = \sum_{\mu=0}^{3} \omega_\mu x^\mu, \tag{1.24}$$

where summation over the repeated upper and lower index μ is implied. This is called a *contraction* of the index μ.
Vector fields $A : \mathbb{M} \to \mathbb{M}$ are given by

$$A(x) = (A^\mu(x)) = (A^0(x), ..., A^3(x)). \tag{1.25}$$

Tensor fields of order (m, n) are defined as maps $T : \mathbb{M} \to (\underbrace{\mathbb{M} \otimes \cdots \mathbb{M}}_{m}) \otimes (\underbrace{\mathbb{M}^* \otimes \cdots \mathbb{M}^*}_{n})$ and their components at a spacetime point x are denoted by

$$T^{\mu_1 \ldots \mu_m}{}_{\nu_1 \ldots \nu_n}(x). \tag{1.26}$$

Linear maps $M : \mathbb{M} \to \mathbb{M}$ can be identified with constant tensor fields of order $(1, 1)$ and their components are denoted by $M^\mu{}_\nu$. The action of M on a vector x is then written as

$$(Mx)^\mu = M^\mu{}_\nu\, x^\nu. \tag{1.27}$$

The composition of linear maps B, C is given as

$$(BC)^\mu{}_\nu = B^\mu{}_\rho\, C^\rho{}_\nu. \tag{1.28}$$

Moreover, we have

$$B^\nu{}_\mu = (B^T)^\mu{}_\nu. \tag{1.29}$$

The transpose thus converts vector indices in covector indices and vice versa.
$M^\mu{}_\mu = \sum_{\mu=0}^{3} M^\mu{}_\mu$ yields the trace of M (sum of diagonal elements).

The *identity map* is denoted by

$$I = (\delta^\mu{}_\nu) \tag{1.30}$$

where $\delta^\mu{}_\nu = 1$ if $\mu = \nu$ and $\delta^\mu{}_\nu = 0$ else.

The *spacetime-metric* should be seen as a (constant) tensor of order $(0,2)$. The components of the inverse of the metric, η^{-1}, are denoted by $\eta^{\mu\nu}$ (note the index placement!) and given by the relation

$$\eta^{\mu\rho}\eta_{\rho\nu} = \delta^{\mu}{}_{\nu}. \tag{1.31}$$

This leads to $\eta^{\mu\nu} = \eta_{\mu\nu}$, i.e., η and η^{-1} have the same components, apart from the index placement.

Using $\eta_{\mu\nu}$ and $\eta^{\mu\nu}$, we introduce the concept of *raising and lowering indices*. For any vector with components x^μ, we define a corresponding covector with components x_μ by:

$$x_\mu = \eta_{\mu\nu}\, x^\nu. \tag{1.32}$$

Concretely, if $(x^\mu) = (x^0, x^1, x^2, x^3)$, then $(x_\mu) = (x^0, -x^1, -x^2, -x^3)$.
Similarly, for a covector with components y_μ, we define a corresponding vector with components y^μ by

$$y^\mu = \eta^{\mu\nu}\, y_\nu. \tag{1.33}$$

Concretely, if $(y_\mu) = (y_0, y_1, y_2, y_3)$, then $(y^\mu) = (y_0, -y_1, -y_2, -y_3)$.
Similarly we define the operators of raising/lowering indices for all tensors. Remember: the index placement is important! It should be clear from the start which index placement an object should have.

Derivatives with respect to coordinates are denoted by

$$\partial_\mu = \frac{\partial}{\partial x^\mu} \tag{1.34}$$

and also here we use $\partial^\mu = \eta^{\mu\nu}\partial_\nu$.

Finally, the *Minkowski square* of a vector $x \in \mathbb{M}$ is defined by:

$$x^2 = x_\mu x^\mu. \tag{1.35}$$

2. The Poincaré group

2.1 Lorentz transformations.

These are the symmetry transformations of Minkowski spacetime.

Definition: A *Lorentz transformation* is a map

$$\Lambda : \mathbb{M} \to \mathbb{M}, \quad x \mapsto \Lambda^{\mu}{}_{\nu}\, x^{\nu} \tag{2.1}$$

which preserves spacetime distances:

$$\forall x, y \in \mathbb{M} : \; s^2(\Lambda x, \Lambda y) = s^2(x, y). \tag{2.2}$$

This is equivalent to

$$\forall x \in \mathbb{M} : \; \eta(\Lambda x, \Lambda x) = \eta(x, x). \tag{2.3}$$

The set of all Lorentz transformations is denoted by $\mathcal{L}$.

Definition: A *real Lie group* is a group G which is also a real, finite-dimensional smooth manifold. In addition, the group operations multiplication and inversion are required to be smooth maps from $G \times G \to G$.

Theorem 2.1.1 *$\mathcal{L}$ is a 6-dimensional Lie group. It is often called $\mathcal{L} = O(3,1)$.*

Proof: → Sheet 2, Exercise 1

Examples.

1. *Rotations.* Let $R \in SO(3)$ be a rotation. $SO(3)$ is the group of orthogonal real 3×3 matrices with determinant equal to 1. This defines a Lorentz transformation by leaving the time coordinate unchanged:

$$\Lambda = \begin{pmatrix} 1 & 0^T \\ 0 & R \end{pmatrix}. \tag{2.4}$$

   Each rotation is characterized by an axis of rotation $\mathbf{n} \in \mathbb{R}^3$ (2 parameters) and an angle φ specifying how far the rotation goes (1 parameter). We shall denote these parameters as $\boldsymbol{\varphi} = \varphi\, \mathbf{n}$.

2. *Boosts.* These describe the transition from the old frame to another moving with velocity $\mathbf{v}$ ($v = |\mathbf{v}| < 1$) with respect to the former. Let

$$\gamma(v) = \frac{1}{\sqrt{1-v^2}}. \tag{2.5}$$

Then the boost is given by

$$\Lambda = \begin{pmatrix} \gamma(v) & \gamma(v)\mathbf{v}^T \\ \gamma(v)\mathbf{v} & \mathbb{1}_3 + \frac{\gamma(v)-1}{v^2}\mathbf{v}\mathbf{v}^T \end{pmatrix}. \tag{2.6}$$

Note: $\mathbf{v}$ should be regarded as a column vector, and $(\mathbf{v}\mathbf{v}^T)_{ij} = v_i v_j$. If we parametrize $\mathbf{v}$ as

$$\mathbf{v} = \tanh(\omega)\,\mathbf{v}/|\mathbf{v}|, \quad \omega \in [0,\infty) \tag{2.7}$$

then every Lorentz boost is characterized by the boost vector

$$\boldsymbol{\omega} = \omega\,\mathbf{v}/|\mathbf{v}| \in \mathbb{R}^3. \tag{2.8}$$

3. *Discrete transformations.* In addition, there are also the space inversion P ("parity"), the time reversal T and the combination of both, PT.

$$P = \begin{pmatrix} 1 & 0^T \\ 0 & -\mathbb{1}_3 \end{pmatrix}, \quad \begin{pmatrix} -1 & 0^T \\ 0 & \mathbb{1}_3 \end{pmatrix}, \quad PT = -\mathbb{1}_4. \tag{2.9}$$

Remark. The Lorentz group consists of the following four connected components:

$$\begin{aligned} \mathcal{L}_+^\uparrow &= \{\Lambda \in \mathcal{L} |\, \Lambda^0{}_0 \geq 1,\ \det\Lambda = +1\}, \\ \mathcal{L}_-^\uparrow &= \{\Lambda \in \mathcal{L} |\, \Lambda^0{}_0 \geq 1,\ \det\Lambda = -1\} = P\mathcal{L}_+^\uparrow, \\ \mathcal{L}_-^\downarrow &= \{\Lambda \in \mathcal{L} |\, \Lambda^0{}_0 \leq -1,\ \det\Lambda = -1\} = T\mathcal{L}_+^\uparrow, \\ \mathcal{L}_+^\downarrow &= \{\Lambda \in \mathcal{L} |\, \Lambda^0{}_0 \leq -1,\ \det\Lambda = +1\} = PT\mathcal{L}_+^\uparrow. \end{aligned} \tag{2.10}$$

The discrete transformations thus relate the connected components of $\mathcal{L}$ to each other. $\mathcal{L}_+^\uparrow$ is called the *proper Lorentz group* and is itself a Lie group.

Visualization of Lorentz boosts: Minkowski diagrams. A boost in x^1 direction is given by ($c = 1$):

$$(x')^0 = \gamma(v)(x^0 - vx^1), \quad (x')^1 = \gamma(v)(x^1 - vx^0), \quad ,(x')^2 = x^2, \quad (x')^3 = x^3. \tag{2.11}$$

This change of coordinates can be represented graphically in Minkowski diagrams (see Fig. 2.1).

2.2 Poincaré transformations

Definition: A *Poincaré transformation* $\Pi = (a, \Lambda)$ with $a \in \mathbb{M}$ and $\Lambda \in \mathcal{L}$ is a map $\mathbb{M} \to \mathbb{M}$ defined by

$$\Pi\, x = a + \Lambda x. \tag{2.12}$$

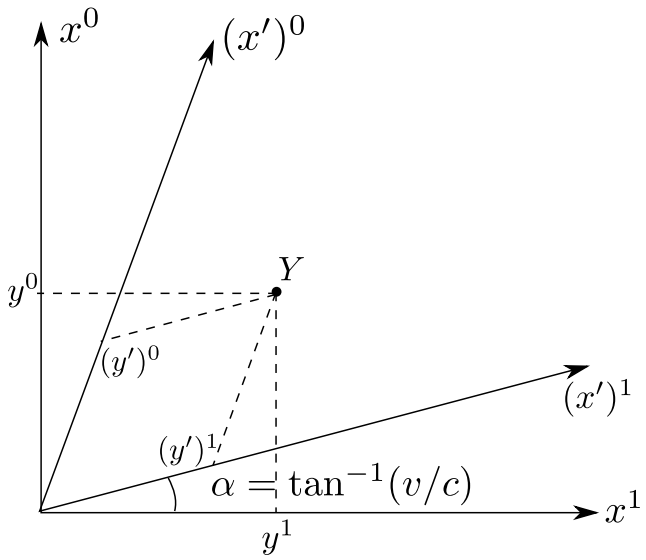

Figure 2.1: Minkowski diagram

Remark. The set $\mathcal{P}$ of Poincaré transformations together with the composition law

$$(a_1, \Lambda_1)(a_2, \Lambda_2) = (a_1 + \Lambda_1 a_2, \Lambda_1 \Lambda_2) \tag{2.13}$$

is a 10-dimensional Lie group.

Transformation laws.

Definition: We call a map $\phi : \mathbb{M} \to \mathbb{R}$ a *scalar field* if it transforms under Poincaré transformation $x \to x' =$ as

$$\phi(x) \to \phi'^{\mu}(x') = \phi(x). \tag{2.14}$$

A map $\phi : \mathbb{M} \to \mathbb{M}$ is called a *vector field* if it transforms as

$$A^{\mu}(x) \to (A')^{\mu}(x') = \Lambda^{\mu}{}_{\nu}\, A^{\nu}(x). \tag{2.15}$$

A *covector field* $\omega : \mathbb{M} \to \mathbb{M}^*$ is defined by

$$\omega_{\mu}(x) \to \omega'_{\mu}(x') = (\Lambda^{-1})^{\nu}{}_{\mu}\, \omega_{\nu}(x). \tag{2.16}$$

Finally, tensor fields are defined to transform according to the vector transformation law for each vector (upper) index and the covector law for each covector (lower) index.

Lie algebra of the Poincaré group.

Definition: 1. The *Lie algebra* $\mathscr{A}$ of an n-dimensional real matrix group G is given by:

$$\mathscr{A} = \{X \in \mathbb{C}^{n\times n} : \forall t \in \mathbb{R} : \exp(tX) \in G\}, \tag{2.17}$$

together with the commutator $[\cdot,\cdot] : \mathscr{A} \times \mathscr{A} \to \mathscr{A}$, $[A, B] = AB - BA$.

2. An element $A \in \mathscr{A}$ is called a *generator* of $\mathscr{A}$ if the smallest subalgebra of $\mathscr{A}$ containing A is $\mathscr{A}$ itself.

Generators of the Poincaré group. $\mathcal{P}$ is a 10-dimensional Lie group, so we can introduce coordinates in $\mathbb{R}^{10}$ such that the identity element e corresponds to the origin, and every other element in a neighborhood of e is characterized by

$$q = (a, \boldsymbol{\omega}, \boldsymbol{\varphi}) \in \mathbb{R}^{10}. \tag{2.18}$$

Choosing a as the translation vector, $\boldsymbol{\omega}$ as the boost parameter and $\boldsymbol{\varphi}$ as the rotation parameter, the coordinate lines $q_j(t) = (0, ..., t, ..., 0)$ (j-th place) are one-parameter subgroups of the proper Poincaré group

$$\mathcal{P}_+^\uparrow = \{(a, \Lambda) \in \mathcal{P} : \Lambda \in \mathcal{L}_+^\uparrow\} \tag{2.19}$$

such that group multiplication is given by adding the parameters as in

$$q_j(s) \circ q_j(t) = q_j(s + t). \tag{2.20}$$

One obtains 10 one-parameter subgroups in this way. Their infinitesimal generators A_j are defined by

$$A_j = \frac{d}{dt} q_j(t)\Big|_{t=0} \tag{2.21}$$

and denoted as follows:

$-p_0 = -H_0$	generator of x^0-translations,
p_1, p_2, p_3	generators of x^1, x^2, x^3-translations,
$-N_1, -N_2, -N_3$	generators of boosts in x^1, x^2, x^3-directions,
J_1, J_2, J_3	generators of rotations around the x^1, x^2, x^3-axes.

Their Lie algebra is given by:

$$[p_j, p_k] = 0 = [p_j, H_0] = [J_j, H_0],$$
$$[N_j, p_k] = -\delta_{jk} H_0, \qquad [N_j, H_0] = p_j,$$
$$[J_j, p_k] = -\sum_m \varepsilon_{jkm} p_m \qquad [J_j, J_k] = -\sum_m \varepsilon_{jkm} J_m,$$
$$[N_j, N_k] = \sum_m \varepsilon_{jkm} J_m \qquad [J_j, N_k] = -\sum_m \varepsilon_{jkm} N_m.$$

Note: The last three equations form the Lie algebra of the Lorentz group.

Index notation for generators. We can conveniently summarize the Poincaré Lie algebra as follows. Let

$$M^{j0} = N_j, \ j = 1, 2, 3, \quad M^{12} = J_3, \quad M^{13} = J_2, \quad M^{23} = J_1 \tag{2.22}$$

and define $M^{\nu\mu} = -M^{\mu\nu}$, $\mu\nu = 0, 1, 2, 3$. Then the Poincaré Lie algebra is given by:

$$[M_{\mu\nu}, p_\sigma] = i(\eta_{\nu\sigma} p_\mu - \eta_{\mu\sigma} p_\nu), \tag{2.23}$$

$$[p_\mu, p_\nu] = 0 \tag{2.24}$$

and

$$[M_{\mu\nu}, M_{\rho\sigma}] = -i(\eta_{\mu\rho} M_{\nu\sigma} - \eta_{\nu\rho} M_{\mu\sigma} + \eta_{\mu\sigma} M_{\rho\nu} - \eta_{\nu\sigma} M_{\rho\mu}). \tag{2.25}$$

Exponentiating the Lie algebra. We obtain the proper Poincaré group $\mathcal{P}_+^\uparrow$ through exponentiation as

$$\mathcal{P}_+^\uparrow = \{\exp(i p_\mu a^\mu) \exp(\omega_{\mu\nu} M^{\mu\nu}/2) : a^\mu \mathbb{R} \, \forall \mu, \ \omega_{\mu\nu} \in \mathbb{R}, \ \omega_{\mu\nu} = -\omega_{\nu\mu} \, \forall \mu, \nu\}. \tag{2.26}$$

Example. The generator of boosts in x^1-direction is given by:

$$N_1 = -\begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{pmatrix}. \tag{2.27}$$

Through exponentiation, we obtain:

$$\exp(N_1\omega) = \sum_{k=0}^{\infty} \frac{(N_1\omega)^k}{k!} = \sum_{k=0}^{\infty} \frac{(N_1\omega)^{2k}}{(2k)!} + \sum_{k=0}^{\infty} \frac{(N_1\omega)^{2k+1}}{(2k+1)!} \tag{2.28}$$

$$= \begin{pmatrix} \cosh\omega & -\sinh\omega & 0 & 0 \\ -\sinh\omega & \cosh\omega & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}. \tag{2.29}$$

Identifying the parameter ω ("rapidity") with

$$\beta = \tanh^{-1}(v), \quad v < 1 \tag{2.30}$$

yields $\cosh\omega = \gamma(v)$ and $\sinh\omega = v\gamma(v)$. Thus we re-obtain the previous form of Lorentz boosts.

Infinitesimal Poincaré transformations. By Taylor expanding (2.26), we obtain the infinitesimal version of a Poincaré transformation as:

$$\Lambda x + a = \left(\mathbb{1} + \frac{1}{2}\omega_{\mu\nu}M^{\mu\nu}\right)x + a \tag{2.31}$$

where now $|\omega^{\mu\nu}|, |a^\mu| \ll 1$ is assumed for all $\mu\nu$.

2.3 Invariance of wave equations

Consider a linear partial differential equation (oder possibly also pseudo-differential equation, see later) of the form

$$D_x\psi(x) = 0 \tag{2.32}$$

where D_x is a differential operator and $\psi(x)$ comes from some vector space V, e.g. $V = C^\infty(\mathbb{R}^4, \mathbb{C}^k)$. k is the number of components of ψ.

Definition: A *representation* of a group G on a vector space V (the *representation space*) over a field $\mathbb{K}$ is a map

$$\rho : G \to GL(V), \tag{2.33}$$

where $GL(V)$ is the group of invertible linear maps $V \to V$, such that

(i) For the identity element $e \in G$:

$$\rho(e) = \mathbb{1}_V \quad \text{(identity on } V\text{)}, \tag{2.34}$$

(ii)

$$\rho(g_1 g_2) = \rho(g_1)\rho(g_2) \ \forall g_1, g_2 \in G. \tag{2.35}$$

In the case that V is finite dimensional, we let $n = \dim V$ and identify $GL(V)$ with $GL(n, \mathbb{K})$, the group of $n \times n$ invertible matrices on the field $\mathbb{K}$. In that case, we call ρ a *matrix representation.*

If V is a complex vector space equipped with a scalar product $\langle \cdot, \cdot \rangle$ then we call the representation ρ *unitary* if all $\rho(g)$ are unitary for all $g \in G$. (Similarly for antiunitary.)

If V is a Hilbert space and G a topological group, then we call ρ a *Hilbert space representation* if in addition to (i), (ii):

(iii) $g_n \to g$ in G implies for all $\psi \in V$: $\rho(g_n)\psi \to \rho(g)\psi$ (strong continuity).

Two representations ρ, π on V are said to be *equivalent* if there is an isomorphism $\phi : V \to V$ such that for all $g \in G$:

$$\phi \circ \rho(g) \circ \phi^{-1} = \pi(g). \tag{2.36}$$

Definition: Equation (2.32) is called *invariant* under a matrix representation ρ of a group G on the representation space $\mathbb{C}^k$ if for every solution ψ of (2.32) and every $g \in G$ also the transformed wave function

$$\psi'(x') = \rho(g)\psi(x) \tag{2.37}$$

is a solution of (2.32) in the variables $x' = gx$.

Remark. Invariance under a matrix representation is only a minimal requirement. Often additional requirements are appropriate, such as the invariance under a unitary representation. Furthermore, one often seeks a representation on a Hilbert space instead of just a matrix representation. We shall discuss what kind of representation one can obtain case-by-case for the individual wave equations we shall study in the lecture.

2.4 Wish list for a relativistic wave equation

1. Linear partial differential equation
2. Invariant under a representation of the Poincare group
3. Implies a continuity equation for a 4-current $j = (\rho, \mathbf{j})$
4. j is future-pointing and time-like, i.e. $j_\mu j^\mu > 0$, $j^0 > 0$,
5. j^0 reduces to $|\psi|^2$ in a suitable non-relativistic limit (or $j^0 = |\psi|^2$ in general)
6. The equation has propagation speed < 1, meaning that the support of solutions grows with at most the speed of light.

3. The Klein-Gordon equation

3.1 Derivation

Recall the quantization recipe for the Schrödinger equation. The idea was to take the energy-momentum relation and to replace E and p by operators. This recipe is applicable to the relativistic case as well. The relativistic energy-momentum relation reads

$$E = \sqrt{\mathbf{p}^2c^2 + m^2c^4}. \tag{3.1}$$

Using the quantization recipe $E \to i\hbar\partial_t$ and $\mathbf{p} \to -i\hbar\nabla$ leads to the so-called *Salpeter equation*

$$i\hbar\partial_t\psi(t,\mathbf{x}) = \sqrt{-\nabla^2\hbar^2c^2 + m^2c^4}\,\psi(t,\mathbf{x}). \tag{3.2}$$

This equation can be understood as a pseudo-differential equation for scalar wave function $\psi : \mathbb{M} \to \mathbb{C}$ which are also square integrable (L^2) with respect to $\mathbf{x}$. The idea is to use the Fourier transformation to define what the operator $\sqrt{\mathbf{p}^2c^2 + m^2c^4}$ means, namely (denoting the spatial Fourier transformation of ψ with $\widetilde{\psi}$):

$$\sqrt{\nabla^2\hbar^2c^2 + m^2c^4}\,\psi(t,\mathbf{x}) = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\, e^{i\mathbf{k}\cdot\mathbf{x}}\sqrt{\mathbf{k}^2\hbar^2c^2 + m^2c^4}\,\widetilde{\psi}(t,\mathbf{k}). \tag{3.3}$$

The Fourier transformation implies that (3.2) has a non-local feature, meaning that the evaluation $\sqrt{-\nabla^2\hbar^2c^2 + m^2c^4}\psi(t,\mathbf{x})$ in a point $(t,\mathbf{x})$ requires the knowledge of $\widetilde{\psi}(t,\mathbf{k})$ for all $\mathbf{k} \in \mathbb{R}^3$ (and thus of $\psi(t,\mathbf{x})$ for all $\mathbf{x}$). The Salpeter equation thus does not treat space and time on an equal level: the time derivative occurs as an ordinary partial derivative while the spatial derivatives occur as a pseudo-differential operator. It is, however, still possible to prove the relativistic invariance using the trivial representation of the (proper) Poincaré group $\rho(a,\Lambda) = 1\ \forall(a,\lambda) \in \mathcal{P}_+^\uparrow$, i.e., with the transformation rule

$$\psi'(x') = \psi(x). \tag{3.4}$$

A major problem, though, is the fact that $|\psi|^2$ cannot be the 0-component of a current 4-vector that transforms in the right way. This is because then $|\psi|^2$ would have to transform as the component of a vector while in fact it transforms as a scalar field. (Note that this is a general point which does not depend on the particular wave equation under discussion.) Nevertheless, one can show (**Sheet 3, Exercise 1**) that the integral $P(t) = \int d^3\mathbf{x}\,|\psi|^2(t,\mathbf{x})$ does not depend on time.

Apart from this, (3.2) has an infinite propagation speed (not a propagation speed of at most the speed of light), meaning that after a small time $t >$ a compactly supported wave function $\psi(t,\cdot)$ can have support all over space. For these reasons,

one usually rejects the Salpeter equation as a relativistic quantum mechanical wave equation.

An obvious way to avoid the pseudo-differential equation (3.2) is to take the square of the energy momentum relation,

$$E^2 = \mathbf{p}^2c^2 + m^2c^4 \tag{3.5}$$

and to only then apply the quantization recipe. This leads to the *Klein-Gordon (KG) equation*:

$$-\partial_t^2\hbar^2\psi(t,\mathbf{x}) = (-\nabla^2\hbar^2c^2 + m^2c^4)\psi(t,\mathbf{x}). \tag{3.6}$$

A more compact way of writing the equation is (after dividing by $c^2\hbar^2$):

$$\left(\Box + \frac{m^2c^2}{\hbar^2}\right)\psi(t,\mathbf{x}) = 0 \tag{3.7}$$

where

$$\Box = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \Delta \tag{3.8}$$

is the d'Alembertian (also called "wave operator").

In index notation, the KG equation can also be expressed as

$$\left(\partial_\mu\partial^\mu + \frac{m^2c^2}{\hbar^2}\right)\psi(t,\mathbf{x}) = 0. \tag{3.9}$$

From now on, we shall again set $\hbar = 1 = c$.

3.2 Physical properties

Relativistic invariance.

Theorem 3.2.1 *The KG equation is invariant under the trivial representation of the Poincaré group*

$$\rho(g) = 1 \ \forall g \in \mathcal{P}. \tag{3.10}$$

The proof is an immediate consequence of **Sheet 2, Exercise 1** where you will show that $\partial_\mu\partial^\mu f$ transforms, for every scalar function $f : \mathbb{M} \to \mathbb{C}$, as a scalar under Lorentz transformations $\Lambda : x \mapsto x' = \Lambda x$, meaning that

$$\partial'_\mu\partial^{\mu'}\phi'(x') = \partial_\mu\partial^\mu\phi(x). \tag{3.11}$$

For a Poincaré transformation $(a,\Lambda) : x \mapsto x' = \Lambda x + a$, the transformation behavior is the same as the operator ∂_μ is invariant under translations. Moreover, the mass term transforms by definition as

$$m^2\phi'(x') = m^2\phi(x). \tag{3.12}$$

Thus, the whole KG equation is Poincaré invariant.

Plane wave solutions. We make the ansatz

$$\phi(x) = e^{-ik_\mu x^\mu} \tag{3.13}$$

where $k^0 = E$. Inserting (3.13) into the KG equation yields

$$(-k^2 + m^2)e^{-ik_\mu x^\mu} = 0. \tag{3.14}$$

Hence we obtain a plane-wave solution if the following *dispersion relation* holds:

$$k^2 = m^2 \quad \Leftrightarrow \quad (k^0)^2 \ (= E^2) = \mathbf{k}^2 + m^2. \tag{3.15}$$

Let

$$\omega(\mathbf{k}) = \sqrt{\mathbf{k}^2 + m^2}. \tag{3.16}$$

At this point, we see an important feature of the KG equation: **For every $\mathbf{k} \in \mathbb{R}^3$, both $E = +\omega(\mathbf{k})$ and $E = -\omega(\mathbf{k})$ lead to a plane-wave solution.** The meaning of negative energies is unclear at this point. It is certainly something one it not used to from classical physics or from non-relativistic QM where the Hamiltonian is bounded from below so that one can make all energies positive by addition of a constant. If this is not the case, one might for example worry that the system could lower its energy indefinitely by emitting radiation (which does not happen in nature). However, these are just worries which are based on an intuition comes from equations different from the KG equation. We have to analyze the KG equation deeper to see whether negative energies are really problematic.

For the moment, we note that for $\widetilde{\phi}_+, \widetilde{\phi}_- \in C(\mathbb{R}^3, \mathbb{C}) \cap L^2(\mathbb{R}^3, \mathbb{C})$ we obtain a large class of solutions of the KG equation by (inverse) Fourier transformation as:

$$\psi(x) = \int \frac{d^3\mathbf{k}}{(2\pi)^3} \left(e^{i\mathbf{k}\cdot\mathbf{x} - i\omega(\mathbf{k})x^0} \widetilde{\phi}_+(\mathbf{k}) + e^{i\mathbf{k}\cdot\mathbf{x} - i\omega(\mathbf{k})x^0} \widetilde{\phi}_-(\mathbf{k}) \right). \tag{3.17}$$

Conserved current. One can check (**Sheet 3, Exercise 2**) that for every differentiable solution $\psi(x)$ of the KG equation the current

$$j^\mu(x) = \mathrm{Im}\left(\psi(x)\partial^\mu\psi^*(x)\right) \tag{3.18}$$

is conserved, meaning

$$\partial_\mu j^\mu(x) = 0. \tag{3.19}$$

Furthermore, it follows from **Sheet 2, Exercise 1** that j transforms under Poincaré transformations as a vector field, i.e.

$$j'^\mu(x') = \Lambda^\mu{}_\nu j^\nu(x). \tag{3.20}$$

However, there is a disturbing property of the density component

$$\rho(t, \mathbf{x}) = j^0(t, \mathbf{x}) = \mathrm{Im}\left(\psi(t, \mathbf{x})\partial_t\psi^*(t, \mathbf{x})\right), \tag{3.21}$$

namely $\rho(t, \mathbf{x})$ **can become negative for certain wave functions** $\psi(t, \mathbf{x})$**.** For example, consider a plane wave solution with negative energy $E = -\omega(\mathbf{k})$ for some $\mathbf{k} \in \mathbb{R}^3$:

$$\psi(t, \mathbf{x}) = e^{i\mathbf{k}\cdot\mathbf{x} + i\omega(k)t}. \tag{3.22}$$

Then:

$$\begin{aligned}\rho(t,\mathbf{x}) &= \mathrm{Im}\left(e^{i\mathbf{k}\cdot\mathbf{x}+i\omega(k)t}\partial_t e^{-i\mathbf{k}\cdot\mathbf{x}-i\omega(k)t}\right)\\ &= \mathrm{Im}\left(e^{i\mathbf{k}\cdot\mathbf{x}+i\omega(k)t}(-i\omega(\mathbf{k}))e^{-i\mathbf{k}\cdot\mathbf{x}-i\omega(k)t}\right)\\ &= -\omega(\mathbf{k}) < 0. \end{aligned} \tag{3.23}$$

Note that we cannot remove this problem by changing the overall sign of j as then a positive energy plane wave would lead to $\rho(t,\mathbf{x}) < 0$. Thus ρ **cannot play the role of a probability density.** The physical interpretation of the KG equation is thus unclear. The source of the problem is the occurrence of both positive and negative energies.

Restriction to positive energies. In view of the above situation, it looks like a logical step to try to restrict oneself to positive energies. That means, we only admit solutions of the form

$$\psi(x) = \int \frac{d^3\mathbf{k}}{(2\pi)^3}\, e^{i\mathbf{k}\cdot\mathbf{x}-i\omega(\mathbf{k})x^0}\widetilde{\phi}_+(\mathbf{k}). \tag{3.24}$$

for some function $\phi_+ \in L^2(\mathbb{R}^3)$. Such a $\psi(t,\mathbf{x})$ also solves the Salpeter equation. We call the vector space of solutions of the form (3.24) V_{pos}.

The situation can then be summarized as follows.

1. The "total probability integral"

$$P(\Sigma) = \int_\Sigma d\sigma_\mu(x)\,\mathrm{Im}(\psi(x)\partial^\mu\psi^*(x)) \tag{3.25}$$

   is, for every space-like hyperplane $\Sigma \subset \mathbb{M}$, positive and independent of Σ. (This can be seen by first specializing to the case of $\Sigma = \Sigma_t = \{(t,\mathbf{x}) \in \mathbb{M} : t = \mathrm{const}\}$ and using (3.24). In a second step one can then employ the result of Exercise 3, Sheet 2 to show that the result holds for all space-like hyperplanes Σ. $\rightarrow$ **Sheet 3, Exercise 2**.)

2. Nevertheless, $j^\mu(x) = \mathrm{Im}(\psi(x)\partial^\mu\psi^*(x))$ can be space-like for certain wave functions ψ.[1]

3. The restriction to positive energies does not work anymore if one includes an external potential in the KG equation. This would be done (according to the quantization recipe) as:

$$(E_{\mathrm{kin}}+V)^2 = \mathbf{p^2}+\mathbf{m^2} \quad\rightarrow\quad (-\partial_t+V)^2\psi(t,\mathbf{x}) = (-\nabla^2+m^2)\psi(t,\mathbf{x}). \tag{3.26}$$

   A potential can then cause transitions from positive to negative energies.

Overall, a probabilistic interpretation of the KG equation is thus problematic, and we shall later look for a different wave equation. However, as the KG equation is still used as a toy example (and also as an ingredient for some quantum field theories), we shall now study its mathematical theory first.

[1] See R. Tumulka, J. Phys. A: Math. Gen. 35 (2002) 7961-7962, `https://arxiv.org/abs/quant-ph/0202140`. $\rightarrow$ **Sheet 3, Exercise 2**.

3.3 Solution theory

Green's function method for the initial boundary value problem. We follow Zauderer[2]. For a bounded region $G \subset \mathbb{R}^3$ and the time interval $[0,T]$, we would like to solve the boundary initial value problem

$$\begin{cases} \psi(0,\mathbf{x}) = f(\mathbf{x}), & \mathbf{x} \in G, \\ \partial_t \psi(0,\mathbf{x}) = g(\mathbf{x}), & \mathbf{x} \in G, \\ \psi(t,\mathbf{x}) = B(t,\mathbf{x}), & \mathbf{x} \in \partial G,\ t \in [0,T] \\ (\Box + m^2)\psi(t,\mathbf{x}) = 0, & \mathbf{x} \in G,\ t \in [0,T]. \end{cases} \tag{3.27}$$

Here, f, g and B are given functions. We may (where necessary) assume them to be smooth in order to avoid technical complications. Note that in (3.27) we have to prescribe $\partial_t \psi 0, \cdot)$ in addition to $\psi(0,\cdot)$. This is because the KG equation is of second order.

Here we consider a bounded region as an intermediary step. The result for unbounded regions is obtained in a suitable limit. The exact form of the boundary conditions then does not matter. Here we we chose Dirichlet boundary conditions.

The idea is to use an integral theorem for a cleverly chosen combination of functions as well as for the spacetime region

$$R = G \times [0,T] \tag{3.28}$$

for some $T > 0$. The boundary of R has the form

$$\partial R = \partial R_0 \cup \partial R_T \cup \partial R_{\mathbf{x}} \tag{3.29}$$

where $\partial R_0 = \{(t,\mathbf{x}) \in \partial R : t = 0\}$, $\partial R_T = \{(t,\mathbf{x}) \in \partial R : t = T\}$ and $\partial R_{\mathbf{x}} = \{(t,\mathbf{x}) \in \partial R : \mathbf{x} \in \partial G\}$. The exterior unit normal vector n at ∂R has the form $n = (-1,\mathbf{0})$ on ∂R_0, $n = (1,\mathbf{0})$ on ∂R_T and $n = (0,\mathbf{n}_x)$ on $\partial R_{\mathbf{x}}$.

We furthermore write the KG equation as

$$\partial_t^2 \psi(t,\mathbf{x}) = -(-\Delta + m^2)\psi(t,\mathbf{x}) =: -L\psi(t,\mathbf{x}). \tag{3.30}$$

Now we come to the integral identity. For arbitrary differentiable functions $u(t,\mathbf{x}), w(t,\mathbf{x})$ we have,

$$\begin{aligned} \partial_\mu(w\partial^\mu u - u\partial^\mu w) &= (\partial_\mu w)(\partial^\mu u) + w\Box u - (\partial_\mu u)(\partial^\mu w) - u\Box w = w\Box u - u\Box w \\ &= w\partial_t^2 u - w\Delta u - w\partial_t^2 u + u\Delta w - wm^2 u + um^2 w \\ &= w(\partial_t^2 u + Lu) - u(\partial_t^2 w + Lw). \end{aligned} \tag{3.31}$$

Therefore we find, using the 4-dimensional divergence theorem applied to the vector field $w\partial^\mu u - u\partial^\mu w$:

$$\int_R dt\, d^3\mathbf{x}\, [w((\partial_t^2 u) + Lu) - u((\partial_t^2 w) + Lw)] = \int_{\partial R} d\sigma\, n_\mu (w\partial^\mu u - u\partial^\mu w). \tag{3.32}$$

[2]E. Zauderer, Partial Differential Equations of Applied Mathematics, Wiley 2006, pp. 412

Here we have:

$$\int_{\partial R} d\sigma\, n_\mu (w\partial^\mu u - u\partial^\mu w)$$
$$= \int_{\partial R_{\mathbf{x}}} d\sigma\, (-w\nabla u + u\nabla w)\cdot \mathbf{n} + \int_{\partial R_T} d\sigma\, (w\partial_t u - u\partial_t w) - \int_{\partial R_0} d\sigma\, (w\partial_t u - u\partial_t w). \tag{3.33}$$

The idea of the Green's function method now is to choose a particular function w such that $u(\tau, \mathbf{y})$ can be determined from (3.33) at a particular point $(\tau, \mathbf{y}) \in R$. It turns out that w will then in general be a generalized function (distribution). The following manipulations will therefore only be of formal nature, and we have to check in the end whether we really obtain a sensible solution. We require:

$$\partial_t^2 w(t, \mathbf{x}) + Lw(t, \mathbf{x}) = \delta(t-\tau)\delta^{(3)}(\mathbf{x}-\mathbf{y}). \tag{3.34}$$

Then:

$$\int_R d^4x\, u(\partial_t^2 w + Lw) = \int_R d^4x\, u\, \delta(t-\tau)\delta^{(3)}(\mathbf{x}-\mathbf{y}) = u(\tau, \mathbf{y}). \tag{3.35}$$

For a solution u of the KG equation we have:

$$\int_R d^4x\, w(\partial_t^2 u + Lu) = 0, \tag{3.36}$$

so the l.h.s. of (3.32) reduces to $u(\tau, \mathbf{y})$. We now work at simplifying the r.h.s.

Furthermore, we have:

$$\int_{\partial R_{\mathbf{x}}} d\sigma\, (-w\nabla u + u\nabla w)\cdot \mathbf{n} = \int_{\partial R_{\mathbf{x}}} d\sigma \left(-w\frac{\partial u}{\partial n} + u\frac{\partial w}{\partial n}\right). \tag{3.37}$$

Thus, if we require

$$w(t, \mathbf{x})|_{\partial R_{\mathbf{x}}} = 0 \tag{3.38}$$

then we find, using both the boundary conditions for w $(= 0)$ and u $(= B)$:

$$\int_{\partial R_{\mathbf{x}}} d\sigma \left(-w\frac{\partial u}{\partial n} + u\frac{\partial w}{\partial n}\right) = \int_{\partial R_{\mathbf{x}}} d\sigma\, B\frac{\partial w}{\partial n}. \tag{3.39}$$

Here, $\frac{\partial w}{\partial n} = \mathbf{n}\cdot\nabla w$ denotes the normal derivative of w (in the spatial directions).

In order to determine w completely, we expect that initial conditions for w and w_t must be prescribed for some t. As we want to utilize (3.33) as best as possible, we have to examine at which time it makes most sense to prescribe the initial conditions. We want to do this in a way such that the r.h.s. of (3.33) does not contain any unkown functions. Considering the terms on the r.h.s. of (3.33), we have two possible choices: $t = 0$ or $t = T$. If we prescribe w and $\partial_t w$ for $t = 0$, then the second term in (3.33) still contains $u(t, \mathbf{x})$ and $\partial_t u(t\,\mathbf{x})$ for $t = T$. However, if we prescribe w and $\partial_t w$ for $t = T$ as

$$w(T, \cdot) = 0, \quad \partial_t w(T, \cdot) = 0 \tag{3.40}$$

then the r.h.s. of (3.33) only contains the initial data and boundary values for u. So this is a distinguished choice, and we shall make it. The function w defined by the conditions (3.34), (3.38) and (3.40) is called the *Green's function* for the initial boundary value problem, and it is denoted by

$$K(t,\mathbf{x};\tau,\mathbf{y}) = w(t,\mathbf{x}). \tag{3.41}$$

Given a distribution which satisfies these conditions (it may not always exist), we obtain the solution $u(\tau,\mathbf{y})$ through the formula (3.33) as:

$$u(\tau,\mathbf{y}) = \int_{\partial R_0} d\sigma\,(Kg - (\partial_t K)f) - \int_{\partial R_{\mathbf{x}}} d\sigma\, B\frac{\partial K}{\partial n} \tag{3.42}$$

This useful formula gives a solution of the initial boundary value problem, provided the integrals exist (and are of the desired regularity). We will prove this later.

Unbounded domains. We would like to consider the unbounded spatial domain $\mathbb{R}^3$. We achieve this by considering $R = B_r(0)$ and letting $r \to \infty$ in (3.42). This is possible only if the integral

$$\int_{\partial R_0} d\sigma\,(Kg - K_t f) = \int_{B_r(0)} d^3\mathbf{x}\;(K(0,\mathbf{x};\tau,\mathbf{y})g(\mathbf{x}) + (\partial_t K)(0,\mathbf{x};\tau,\mathbf{y})f(\mathbf{x})) \tag{3.43}$$

exists in the limit $r \to \infty$. The second integral in (3.42) can be made identically zero by choosing $B = 0$. Then we have:

$$u(\tau,\mathbf{y}) = \int d^3\mathbf{x}\,(K(0,\mathbf{x};\tau,\mathbf{y})g(\mathbf{x}) - (\partial_t K)(0,\mathbf{x};\tau,\mathbf{y})f(\mathbf{x}))\,. \tag{3.44}$$

Green's function of the KG equation. It is quite some work to calculate the Green's function of the KG equation. A systematic way is to use the Fourier transformation (taking into account the boundary conditions). Another way is to make a suitable ansatz for K, e.g., that K is only a function of the spacetime distance $s^2(t,\mathbf{x};t',\mathbf{x}')$, and thereby reduce the problem to finding singular solutions to an ODE. The result for K is:

$$\begin{aligned} K(t,\mathbf{x};t',\mathbf{x}') &= \frac{1}{4\pi}\frac{\delta(t'-t-|\mathbf{x}'-\mathbf{x}|)}{|\mathbf{x}'-\mathbf{x}|} \\ &- \frac{m}{4\pi}\theta(t'-t-|\mathbf{x}'-\mathbf{x}|)\frac{J_1(m\sqrt{(t'-t)^2-|\mathbf{x}'-\mathbf{x}|^2})}{\sqrt{(t'-t)^2-|\mathbf{x}'-\mathbf{x}|^2}}. \end{aligned} \tag{3.45}$$

Here, J_1 is a Bessel function of the first kind. In general, we have for $n \in \mathbb{N}_0$:

$$J_n(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(k+n)!}\left(\frac{x}{2}\right)^{2k+n} \tag{3.46}$$

Note that

$$\frac{J_1(x)}{x} = \frac{1}{2}\sum_{k=0}^{\infty} \frac{(-1)^k}{k!(k+1)!}\left(\frac{x}{2}\right)^{2k} \tag{3.47}$$

defines a smooth function on $\mathbb{R}$.

K can be written in terms of 4-vectors as:

$$K(x;x') = \frac{1}{2\pi}\theta(x'^0 - x^0)\delta((x'-x)^2) - \frac{m}{4\pi}\theta(x'^0 - x^0)\theta((x'-x)^2)\frac{J_1(m\sqrt{(x'-x)^2})}{\sqrt{(x'-x)^2}} \tag{3.48}$$

where θ denotes the Heaviside step function.

The fact that K is a Green's function of the KG equation can be checked through elementary (but lengthy) calculations. You may know already that

$$\Box\frac{\delta(t'-t-|\mathbf{x}-\mathbf{x}'|)}{4\pi|\mathbf{x}'-\mathbf{x}|} = \delta(t'-t)\delta^{(3)}(\mathbf{x}'-\mathbf{x}), \tag{3.49}$$

which, in turn, follows from $\Delta\frac{1}{|\mathbf{x}'-\mathbf{x}|} = -4\pi\delta^{(3)}(\mathbf{x}'-\mathbf{x})$. Furthermore, one can show that

$$\begin{aligned} &-\Box\frac{m}{4\pi}\theta(t'-t-|\mathbf{x}-\mathbf{x}'|)\frac{J_1(m\sqrt{(t'-t)^2-|\mathbf{x}'-\mathbf{x}|^2})}{\sqrt{(t'-t)^2-|\mathbf{x}'-\mathbf{x}|^2}} \\ &= -m^2\frac{\delta(t'-t-|\mathbf{x}-\mathbf{x}'|)}{4\pi|\mathbf{x}'-\mathbf{x}|} + \frac{m^3}{4\pi}\theta(t'-t-|\mathbf{x}-\mathbf{x}'|)\frac{J_1(m\sqrt{(t'-t)^2-|\mathbf{x}'-\mathbf{x}|^2})}{\sqrt{(t'-t)^2-|\mathbf{x}'-\mathbf{x}|^2}}. \end{aligned} \tag{3.50}$$

To prove this, one uses (among other things) the identity

$$\Box\frac{J_1(m\sqrt{(t'-t)^2-|\mathbf{x}'-\mathbf{x}|^2})}{\sqrt{(t'-t)^2-|\mathbf{x}'-\mathbf{x}|^2}} = -m^2\frac{J_1(m\sqrt{(t'-t)^2-|\mathbf{x}'-\mathbf{x}|^2})}{\sqrt{(t'-t)^2-|\mathbf{x}'-\mathbf{x}|^2}}. \tag{3.51}$$

From these identities it then follows that K is a Green's function of the KG equation. The fact that K satisfies the initial data $K(T,\mathbf{x};\tau,\mathbf{y}) = 0$, $\partial_t K(T,\mathbf{x};\tau,\mathbf{y}) = 0$ is easy to see, as $\theta(t'-T-|\mathbf{x}-\mathbf{x}'|)$, $\delta(t'-T-|\mathbf{x}-\mathbf{x}'|)$ and $\delta'(t'-T-|\mathbf{x}-\mathbf{x}'|)$ vanish for $t \in (0,T)$.

On **Sheet 4, Exercise 1** you will prove a related statement, namely what the Green's function of the 1+1 dimensional KG equation is.

The solution formula. Knowing the Green's function, we can now use (3.44) to express the solution of the Cauchy problem

$$\begin{cases} \psi(0,\mathbf{x}) = f(\mathbf{x}), & \mathbf{x}\in\mathbb{R}^3, \\ \partial_t\psi(0,\mathbf{x}) = g(\mathbf{x}), & \mathbf{x}\in\mathbb{R}^3, \\ (\Box+m^2)\psi(t,\mathbf{x}) = 0, & \mathbf{x}\in\mathbb{R}^3,\ t\in[0,T]. \end{cases} \tag{3.52}$$

in terms of the initial data. In (3.44), we can write

$$-\int d^3\mathbf{x}\,(\partial_t K)(0,\mathbf{x};\tau,\mathbf{y})f(\mathbf{x}) = \partial_\tau\int d^3\mathbf{x}\,K(0,\mathbf{x};\tau,\mathbf{y})f(\mathbf{x}) \tag{3.53}$$

as $K(t,\mathbf{x};\tau,\mathbf{y})$ depends only on the difference $(t-\tau,\mathbf{x}-\mathbf{y})$. Thus, we obtain:

$$
\begin{aligned}
&u(\tau,\mathbf{y}) \\
&= \int d^3\mathbf{x}\left(\frac{1}{4\pi}\frac{\delta(\tau-|\mathbf{y}-\mathbf{x}|)}{|\mathbf{y}-\mathbf{x}|}g(\mathbf{x}) - \frac{m}{4\pi}\theta(\tau-|\mathbf{y}-\mathbf{x}|)\frac{J_1(m\sqrt{\tau^2-|\mathbf{y}-\mathbf{x}|^2})}{\sqrt{\tau^2-|\mathbf{y}-\mathbf{x}|^2}}g(\mathbf{x})\right) \\
&+ \frac{\partial}{\partial\tau}\int d^3\mathbf{x}\left(\frac{1}{4\pi}\frac{\delta(\tau-|\mathbf{y}-\mathbf{x}|)}{|\mathbf{y}-\mathbf{x}|}f(\mathbf{x}) - \frac{m}{4\pi}\theta(\tau-|\mathbf{y}-\mathbf{x}|)\frac{J_1(m\sqrt{\tau^2-|\mathbf{y}-\mathbf{x}|^2})}{\sqrt{\tau^2-|\mathbf{y}-\mathbf{x}|^2}}f(\mathbf{x})\right)
\end{aligned}
\tag{3.54}
$$

We can simplify this result using spherical coordinates $d^3\mathbf{x} = r^2 dr\, d\Omega_{\mathbf{x}}$. The result is:

$$
\begin{aligned}
u(\tau,\mathbf{y}) = \; & \frac{\tau}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, g(\mathbf{x}+\mathbf{y}) - \frac{m}{4\pi}\int_{B_\tau(0)} d^3\mathbf{x}\,\frac{J_1(m\sqrt{\tau^2-|\mathbf{x}|^2})}{\sqrt{\tau^2-|\mathbf{x}|^2}}g(\mathbf{x}+\mathbf{y}) \\
& + \frac{\partial}{\partial\tau}\left(\frac{\tau}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, f(\mathbf{x}+\mathbf{y}) - \frac{m}{4\pi}\int_{B_\tau(0)} d^3\mathbf{x}\,\frac{J_1(m\sqrt{\tau^2-|\mathbf{x}|^2})}{\sqrt{\tau^2-|\mathbf{x}|^2}}f(\mathbf{x}+\mathbf{y})\right).
\end{aligned}
\tag{3.55}
$$

Here, $B_\tau(0) \subset \mathbb{R}^3$ is the ball with radius τ around the origin.

An important fact about the formula (3.55) is that it only contains integrations of smooth functions over bounded regions. We shall use this fact to check that it indeed yields a solution of the Cauchy problem of the KG equation.

Theorem 3.3.1 *Let $f \in C^3(\mathbb{R}^3)$ and $g \in C^2(\mathbb{R}^3)$. Then the function $u : \mathbb{M} \to \mathbb{C}$ defined by* (3.55) *lies in $C^2(\mathbb{R}^4)$ and it solves the Cauchy problem* (3.52).

Proof: *C^2 property.* $u \in \mathbb{C}^2(\mathbb{R})$ as it is defined by integrals involving only f, g and the smooth function $J_1(x)/x$ over bounded domains.
Initial data. To see what $u(0,\mathbf{x})$ is, we take the limit $\tau \to 0$ in (3.55). The two integrals in the first line go to zero as the integrands are continuous functions and as such have an upper bound, say on $\overline{B}_1(0)$. Similarly, in the second line, the only surviving term is

$$
\frac{1}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, f(\mathbf{y}+\mathbf{x}) \to f(\mathbf{x}) \quad \text{for } \tau \to 0, \tag{3.56}
$$

as it should be. For $\partial_\tau u(0,\mathbf{x})$, only the first term in (3.55) contributes, namely:

$$
\begin{aligned}
&\partial_\tau \frac{\tau}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, g(\mathbf{y}+\mathbf{x}) = \frac{1}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, g(\mathbf{y}+\mathbf{x}) + \frac{\tau}{4\pi}\partial_\tau \int_{|\mathbf{n}|=1} d^2\mathbf{n}\, g(\mathbf{y}+\tau\mathbf{n}) \\
&= \frac{1}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, g(\mathbf{y}+\mathbf{x}) + \frac{\tau}{4\pi}\int_{|\mathbf{n}|=1} d^2\mathbf{n}\, \underbrace{\mathbf{n}\cdot\nabla g(\mathbf{y}+\tau\mathbf{n})}_{\text{bounded}} \\
&\xrightarrow{\tau\to 0}\; g(\mathbf{y}) + 0.
\end{aligned}
\tag{3.57}
$$

So the initial conditions are satisfied.
Solution of the KG equation. Our strategy will be as follows: We first show that the terms without mass, i.e.

$$u_1(\tau,\mathbf{y}) = \underbrace{\frac{\tau}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, g(\mathbf{x}+\mathbf{y})}_{=:u_1^{(g)}(\tau,\mathbf{y})} + \underbrace{\frac{\partial}{\partial\tau}\frac{\tau}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, f(\mathbf{x}+\mathbf{y})}_{=:u_1^{(f)}(\tau,\mathbf{y})} \tag{3.58}$$

satisfy the wave equation $\partial_\tau^2 u_1(\tau,\mathbf{y}) = \Delta u_1(\tau,\mathbf{y})$. Then we show that the terms with mass, i.e.

$$u_2(\tau,\mathbf{y}) = \underbrace{-\frac{m}{4\pi}\int_{B_\tau(0)} d^3\mathbf{x}\,\frac{J_1(m\sqrt{\tau^2-|\mathbf{x}|^2})}{\sqrt{\tau^2-|\mathbf{x}|^2}} g(\mathbf{x}+\mathbf{y})}_{=:u_2^{(g)}(\tau,\mathbf{y})} \underbrace{-\frac{\partial}{\partial\tau}\frac{m}{4\pi}\int_{B_\tau(0)} d^3\mathbf{x}\,\frac{J_1(m\sqrt{\tau^2-|\mathbf{x}|^2})}{\sqrt{\tau^2-|\mathbf{x}|^2}} f(\mathbf{x}+\mathbf{y})}_{=:u_2^{(f)}(\tau,\mathbf{y})} \tag{3.59}$$

satisfy

$$(\partial_\tau^2 - \Delta)u_2(\tau,\mathbf{y}) = -m^2\left(u_1(\tau,\mathbf{y}) + u_2(\tau,\mathbf{y})\right). \tag{3.60}$$

This implies that $u = u_1 + u_2$ solves the KG equation.

We start with $\partial_\tau^2 u_1(\tau,\mathbf{y}) = \Delta u_1(\tau,\mathbf{y})$. As f and g can be chosen independently (and in particular one equal to zero), we treat the terms involving them separately. We have:

$$\begin{aligned}
&\frac{\partial}{\partial\tau}u_1^{(g)}(\tau,\mathbf{y}) = \frac{1}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, g(\mathbf{x}+\mathbf{y}) + \frac{\tau}{4\pi}\frac{\partial}{\partial\tau}\int_{|\mathbf{n}=1|} d^2\mathbf{n}\, g(\tau\mathbf{n}+\mathbf{y})\\
&= \frac{1}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, g(\mathbf{x}+\mathbf{y}) + \frac{\tau}{4\pi}\int_{|\mathbf{n}=1|} d^2\mathbf{n}\,\mathbf{n}\cdot\nabla g(\tau\mathbf{n}+\mathbf{y})\\
&= \frac{1}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, g(\mathbf{x}+\mathbf{y}) + \frac{1}{4\pi\tau}\int_{B_\tau(0)} d^3\mathbf{x}\,\Delta g(\mathbf{x}+\mathbf{y})
\end{aligned} \tag{3.61}$$

Here, we have used the divergence theorem for the transition to the last line. Thus,

$$\begin{aligned}
&\frac{\partial^2}{\partial\tau^2}u_1^{(g)}(\tau,\mathbf{y})\\
&= \frac{1}{4\pi}\int_{|\mathbf{n}=1|} d^2\mathbf{n}\,\mathbf{n}\cdot\nabla g(\tau\mathbf{n}+\mathbf{y}) - \frac{1}{4\pi\tau^2}\int_{B_\tau(0)} d^3\mathbf{x}\,\Delta g(\mathbf{x}+\mathbf{y}) + \frac{1}{4\pi\tau}\frac{\partial}{\partial\tau}\int_{B_\tau(0)} d^3\mathbf{x}\,\Delta g(\mathbf{x}+\mathbf{y})\\
&= \frac{1}{4\pi\tau^2}\int_{B_\tau(0)} d^3\mathbf{x}\,\Delta g(\mathbf{x}+\mathbf{y}) - \frac{1}{4\pi\tau^2}\int_{B_\tau(0)} d^3\mathbf{x}\,\Delta g(\mathbf{x}+\mathbf{y}) + \frac{1}{4\pi\tau}\frac{\partial}{\partial\tau}\int_{B_\tau(0)} d^3\mathbf{x}\,\Delta g(\mathbf{x}+\mathbf{y})\\
&= \frac{1}{4\pi\tau}\frac{\partial}{\partial\tau}\int_{B_\tau(0)} d^3\mathbf{x}\,\Delta g(\mathbf{x}+\mathbf{y}).
\end{aligned} \tag{3.62}$$

On the other hand,

$$\begin{aligned}
&\Delta u_1^{(g)}(\tau,\mathbf{y}) = \frac{\tau}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\,\Delta g(\mathbf{x}+\mathbf{y}) = \frac{1}{4\pi\tau}\int_{\partial B_\tau(0)} d\sigma_{\mathbf{x}}\,\Delta g(\mathbf{x}+\mathbf{y})\\
&= \frac{1}{4\pi\tau}\frac{\partial}{\partial\tau}\int_{B_\tau(0)} d^3\mathbf{x}\,\Delta g(\mathbf{x}+\mathbf{y}).
\end{aligned} \tag{3.63}$$

Here we have used the identity

$$\frac{\partial}{\partial\tau}\int_{B_\tau(0)} d^3\mathbf{x}\, h(\mathbf{x}) = \int_{\partial B_\tau(0)} d\sigma_{\mathbf{x}}\, h(\mathbf{x}). \tag{3.64}$$

Thus, the g-part of u_1 solves the wave equation. For the f-part one can proceed analogously as we can interchange ∂_τ^2 and Δ with the overall ∂_τ-derivative, and as the term otherwise has exactly the same form as the g-term. We have obtained the result that u_1 indeed solves the wave equation.

Next, we turn to the proof of the identity (3.60), $\Box u_2 = -m^2(u_1+u_2)$. We again treat the parts of u_2 involving f and g separately. We start with the g-part. The result for the f-part can then be obtained analogously. We have:

$$\begin{aligned}
\frac{\partial}{\partial\tau}u_2^{(g)}(\tau,\mathbf{y}) &= -\frac{m}{4\pi}\frac{\partial}{\partial\tau}\int_0^\tau dt\, t^2 \int d^2\mathbf{n}\, \frac{J_1(m\sqrt{\tau^2-t^2})}{\sqrt{\tau^2-t^2}} g(t\mathbf{n}+\mathbf{y}) \\
&= -\frac{m}{4\pi}\tau^2 \int d^2\mathbf{n} \underbrace{\left(\frac{J_1(m\sqrt{\tau^2-t^2})}{\sqrt{\tau^2-t^2}}\right)_{t\nearrow\tau}}_{=m/2} g(\tau\mathbf{n}+\mathbf{y}) \\
&\quad - \frac{m}{4\pi}\int_0^\tau dt\, t^2 \int d^2\mathbf{n}\, \partial_\tau \left(\frac{J_1(m\sqrt{\tau^2-t^2})}{\sqrt{\tau^2-t^2}}\right) g(t\mathbf{n}+\mathbf{y}).
\end{aligned} \tag{3.65}$$

Taking another τ-derivative yields:

$$\partial_\tau^2 u_2^{(g)}(\tau,\mathbf{y}) = -\frac{m^2\tau}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, g(\mathbf{x}+\mathbf{y}) \tag{3.66}$$

$$-\frac{m^2\tau^2}{8\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, \frac{\partial g}{\partial n}(\mathbf{x}+\mathbf{y}) \tag{3.67}$$

$$-\frac{m\tau^2}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, \underbrace{\partial_\tau\left(\frac{J_1(m\sqrt{\tau^2-t^2})}{\sqrt{\tau^2-t^2}}\right)_{t\nearrow\tau}}_{=-m^3\tau/8} g(\mathbf{x}+\mathbf{y}) \tag{3.68}$$

$$-\frac{m}{4\pi}\int_{B_\tau(0)} d^3\mathbf{x}\, \partial_\tau^2\left(\frac{J_1(m\sqrt{\tau^2-\mathbf{x}^2})}{\sqrt{\tau^2-\mathbf{x}^2}}\right) g(\mathbf{x}+\mathbf{y}). \tag{3.69}$$

This is to be compared with

$$\Delta_{\mathbf{y}} u_2^{(g)}(\tau,\mathbf{y}) = -\frac{m}{4\pi}\int_{B_\tau(0)} d^3\mathbf{x}\frac{J_1(m\sqrt{\tau^2-\mathbf{x}^2})}{\sqrt{\tau^2-\mathbf{x}^2}}\Delta g(\mathbf{x}+\mathbf{y}). \tag{3.70}$$

To bring this closer to the terms we obtained for $\partial_\tau^2 u_2^{(g)}(\tau,\mathbf{y})$, we make use of the second Green's identity

$$\int_V d^3\mathbf{x}\,\phi\Delta\psi = \int_V d^3\mathbf{x}\,\psi\Delta\phi + \int_{\partial V} d\sigma\left(\phi\frac{\partial\psi}{\partial n} - \psi\frac{\partial\phi}{\partial n}\right). \tag{3.71}$$

This yields:

$$
\begin{aligned}
&-\frac{m}{4\pi}\int_{B_\tau(0)} d^3\mathbf{x}\,\frac{J_1(m\sqrt{\tau^2-\mathbf{x}^2})}{\sqrt{\tau^2-\mathbf{x}^2}}\Delta g(\mathbf{x}+\mathbf{y}) \\
&\quad = -\frac{m}{4\pi}\int_{B_\tau(0)} d^3\mathbf{x}\,\Delta_{\mathbf{x}}\left(\frac{J_1(m\sqrt{\tau^2-\mathbf{x}^2})}{\sqrt{\tau^2-\mathbf{x}^2}}\right) g(\mathbf{x}+\mathbf{y}) \qquad (3.72)\\
&\quad\quad -\frac{m}{4\pi}\int_{\partial B_\tau(0)} d\sigma\,\frac{J_1(m\sqrt{\tau^2-\mathbf{x}^2})}{\sqrt{\tau^2-\mathbf{x}^2}}\mathbf{n}\cdot\nabla_{\mathbf{x}} g(\mathbf{x}+\mathbf{y}) \qquad (3.73)\\
&\quad\quad +\frac{m}{4\pi}\int_{\partial B_\tau(0)} d\sigma\,\mathbf{n}\cdot\nabla_{\mathbf{x}}\left(\frac{J_1(m\sqrt{\tau^2-\mathbf{x}^2})}{\sqrt{\tau^2-\mathbf{x}^2}}\right) g(\mathbf{x}+\mathbf{y}). \qquad (3.74)
\end{aligned}
$$

Next, we find that (3.73) agrees with (3.67) because on $\partial B_\tau(0)$, we have $\mathbf{x}^2=\tau^2$ and

$$\lim_{|\mathbf{x}|\to\tau}\frac{J_1(m\sqrt{\tau^2-\mathbf{x}^2})}{\sqrt{\tau^2-\mathbf{x}^2}} = \frac{m}{2}. \qquad (3.75)$$

Similarly, (3.74) agrees with (3.68) on $\partial B_\tau(0)$, $\mathbf{n}=\mathbf{x}/|\mathbf{x}|$ and

$$\lim_{\mathbf{x}^2\to\tau^2}\frac{\mathbf{x}}{|\mathbf{x}|}\cdot\nabla_{\mathbf{x}}\frac{J_1(m\sqrt{\tau^2-\mathbf{x}^2})}{\sqrt{\tau^2-\mathbf{x}^2}} = \frac{m^3\tau}{8}, \qquad (3.76)$$

as one finds after a short calculation with Bessel functions (e.g. using the defining power series).

Thus:

$$
\begin{aligned}
&(\partial_\tau^2-\Delta_{\mathbf{y}}) =: u_2^{(g)}(\tau,\mathbf{y}) = (3.66)+(3.67)-(3.72)\\
&= -\frac{m^2\tau}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, g(\mathbf{x}+\mathbf{y}) - \frac{m}{4\pi}\int_{B_\tau(0)} d^3\mathbf{x}\,(\partial_\tau^2-\Delta_{\mathbf{x}})\left(\frac{J_1(m\sqrt{\tau^2-\mathbf{x}^2})}{\sqrt{\tau^2-\mathbf{x}^2}}\right) g(\mathbf{x}+\mathbf{y}).
\end{aligned} \qquad (3.77)
$$

Now, we have (as one can show after some calculations with Bessel functions):

$$(\partial_\tau^2-\Delta_{\mathbf{x}})\left(\frac{J_1(m\sqrt{\tau^2-\mathbf{x}^2})}{\sqrt{\tau^2-\mathbf{x}^2}}\right) = -m^2\left(\frac{J_1(m\sqrt{\tau^2-\mathbf{x}^2})}{\sqrt{\tau^2-\mathbf{x}^2}}\right), \quad \tau^2>\mathbf{x}^2. \qquad (3.78)$$

Identifying also $u_1^{(g)}(\tau,\mathbf{y}) = -\frac{\tau}{4\pi}\int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, g(\mathbf{x}+\mathbf{y})$, the conclusion is that

$$(\partial_\tau^2-\Delta_{\mathbf{y}})u_2^{(g)} = -m^2(u_1^{(g)}+u_2^{(g)}). \qquad (3.79)$$

Hence, together with the previous result $(\partial_\tau^2-\Delta_{\mathbf{y}})u_1^{(g)}=0$, we obtain that $u^{(g)}=u_1^{(g)}+u_2^{(g)}$ satisfies the KG equation. The same procedure can be used to show that $u^{(f)}=u_1^{(f)}+u_2^{(f)}$ solves the KG equation as well. Thus $u=u^{(g)}+u^{(f)}$ is indeed a solution of the KG equation. □

Uniqueness of the solution. Next, we show that the solution formula (3.55) yields the only solution of the Cauchy problem (3.27). To this end, we use the *method of energy integrals* (see e.g. Zauderer pp. 398).

Theorem 3.3.2 *Let $u_1, u_2 \in C^2([0,T]\times\mathbb{R}^3)$ be two solutions of the Cauchy problem (3.52) with $u_i(t,\cdot), \partial_\mu u_i(t,\cdot), \partial_\mu\partial_\nu u_i(t,\cdot) \in L^2(\mathbb{R}^3)$ for $i = 1,2$, $\mu,\nu = 0,1,2,3$ and all $t \in [0,T]$. Then: $u_1 = u_2$.*

Proof: Consider the "energy integral"

$$E(t) = \frac{1}{2}\int d^3\mathbf{x}\, \left[|\partial_t u|^2 + |\nabla u|^2 + m^2|u|^2\right]. \tag{3.80}$$

We will show that $\frac{d}{dt}E(t) = 0$ for every solution u of the KG equation with the same requirements as for u_1, u_2 in the theorem. Furthermore, we have $E(t) \geq 0\,\forall t$ and $E(t) = 0 \Rightarrow u(t,\cdot) = 0$. Thus, if $u(0,\cdot) = 0$ then it follows that $u(t,\cdot) = 0\,\forall t$. For $u = u_1 - u_2$, we indeed have $u(0,\cdot) = 0$, as u_1 and u_2 satisfy the same initial data. Thus, $u_1(t,\cdot) = u_2(t,\cdot)\,\forall t \in [0,T]$ follows.

We turn to the proof of $\frac{d}{dt}E(t) = 0$. We have:

$$\frac{d}{dt}E(t) = \frac{1}{2}\int d^3\mathbf{x}\, \left[(\partial_t u^*)\partial_t^2 u + (\nabla\partial_t u^*)\cdot\nabla u + m^2(\partial_t u^*)u\right] + \text{c.c.}, \tag{3.81}$$

where "c.c" denotes the complex conjugate of all the terms before. We would like to bring this into a form where we can use that u satisfies the KG equation. To this end, we need to rewrite the middle term. We have:

$$\nabla\cdot[(\partial_t u^*)\nabla u] = (\nabla\partial_t u^*)\cdot\nabla u + \partial_t u^*\Delta u. \tag{3.82}$$

Hence (note that we need the integrability properties here):

$$\frac{d}{dt}E(t) = \frac{1}{2}\int d^3\mathbf{x}\,(\partial_t u^*)(\partial_t^2 u - \Delta u + m^2 u) + \frac{1}{2}\int d^3\mathbf{x}\,\nabla\cdot[(\partial_t u^*)\nabla u] + \text{c.c.} \tag{3.83}$$

Now we use that u is a solution of the KG equation, so the first integral vanishes. We are left with

$$\begin{aligned}\frac{d}{dt}E(t) &= \lim_{r\to\infty}\frac{1}{2}\int_{B_r(0)} d^3\mathbf{x}\,\nabla\cdot[(\partial_t u^*)\nabla u] + \text{c.c.}\\ &= \lim_{r\to\infty}\frac{1}{2}\int_{\partial B_r(0)} d\sigma\,\mathbf{n}\cdot[(\partial_t u^*)\nabla u] + \text{c.c.}\\ &= 0,\end{aligned} \tag{3.84}$$

as $\partial_\mu u(t,\cdot) \in L^2(\mathbb{R}^3)\,\forall\mu$. □

Remark. E can be written as the spatial integral over the 00-component of the *energy-momentum tensor* of the KG equation:

$$T^{\mu\nu}(x) = \frac{1}{2}\left\{(\partial^\nu\psi(x))^*(\partial^\mu\psi(x)) + (\partial^\mu\psi(x))^*(\partial^\nu\psi(x)) - \eta^{\mu\nu}\left[(\partial_\rho\psi(x))^*(\partial^\rho\psi(x)) - m^2|\psi(x)|^2\right]\right\}. \tag{3.85}$$

Then $T^{\mu\nu}$ is real-valued and we have $T^{\mu\nu} = T^{\nu\mu}$. Moreover, one can check (**Sheet 5, Exercise 4**) that the KG equation implies

$$\partial_\mu T^{\mu\nu} = 0\ \forall\nu = 0,1,2,3. \tag{3.86}$$

Hence the integrals

$$P^\nu(\Sigma) = \int_\Sigma d\sigma(x)\, n_\mu(x) T^{\mu\nu}(x) \tag{3.87}$$

are independent of the choice of the space-like hyperplane Σ. This is another way of seeing that $E(t) = P^0(\Sigma_t)$ does not depend on time. Note also that E cannot play the role of total probability, as it transforms as the component of a vector under Lorentz transformations.

Finite propagation speed.

Definition: We say that the KG equation has *finite propagation speed* if for all initial data $f \in C^3(\mathbb{R}^3)$, $g \in C^2(\mathbb{R}^3)$ which are compactly supported in a ball $B_r(0)$ with radius $r > 0$, also the solution $u(t,\cdot)$ and its first derivative $\partial_t u(t,\cdot)$ are compactly supported in a ball of radius $r + |t|$.

Corollary 3.3.3 *The KG equation has finite propagation speed.*

Proof: This can be read off from the solution formula (3.55) (using that it gives the unique solution of the Cauchy problem (3.52). The detailed proof will be an exercise (**Sheet 5, Exercise 1**). □

4. The Dirac equation

4.1 Derivation

This section largely follows Schweber[1].

The main problem of the Klein-Gordon equation is that the density component of the current can become negative. One can see the reason for this behavior in the fact that the current $j^\mu_{\mathrm{KG}} = \mathrm{Im}(\psi\partial^\mu\psi^*)$ contains derivatives. This, in turn, is a consequence of the fact that the KG equation is of second order.

Therefore, Dirac's idea (1928) was that a relativistic quantum mechanical equation should be of first order, both in time and space derivatives. (The latter is unusual, as the Schrödinger equation contains second order spatial derivatives.) He wrote down the general form of a linear equation which involves ψ as well as its time and space derivatives. At the same time, he admitted that

$$\psi = \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_K \end{pmatrix} \tag{4.1}$$

could have K complex-valued components. He arrived at the following general form of the equation (constants have been inserted with hindsight):

$$\frac{1}{c}\frac{\partial\psi}{\partial t} + \sum_{j=1}^{3} \alpha^j \frac{\partial\psi}{\partial x^j} + \frac{imc}{\hbar}\beta\psi = 0. \tag{4.2}$$

This is the general form of the *Dirac equation.* Here, $\alpha^1, \alpha^2, \alpha^3$ and β are constant complex $K \times K$ matrices. (Their constancy is required to obtain Poincaré invariance.) We still need to determine their possible form (and size K). Dirac did this by imposing the following requirements (compare with our wish list):

1. Eq. (4.2) should imply that there is a spatial current $\mathbf{j}$ such that $\rho = \psi^\dagger\psi = \sum_{l=1}^{K} |\psi_l|^2$ and $\mathbf{j}$ satisfy the continuity equation. Then ρ could play the role of a probability density.

2. Each component of ψ should satisfy the KG equation, as it implies the desired energy-momentum relation $p^2 = m^2c^2$. (This should come out in some way in semi-classical situations, e.g. in scattering theory, and having it hold strictly for plane waves will ensure this.)

[1] S. Schweber: An Introduction to Relativistic Quantum Field Theory. Row Peterson and Company, 1961, Chap. 4

So let us see what these requirements lead to. In order to calculate $\partial_t \rho = \partial_t \psi^\dagger \psi$, it is useful to note down the Hermitian conjugate (complex conjugate and transpose) of (4.2).

$$\frac{1}{c}\frac{\partial \psi^\dagger}{\partial t} + \sum_{j=1}^{3} \frac{\partial \psi^\dagger}{\partial x^j}(\alpha^j)^\dagger - \frac{imc}{\hbar}\psi^\dagger \beta^\dagger = 0. \tag{4.3}$$

Taking the time derivative of $\rho = \psi^\dagger \psi$ then leads to:

$$\frac{1}{c}\partial_t \psi^\dagger \psi = -\sum_{j=1}^{3} \left(\frac{\partial \psi^\dagger}{\partial x^j}(\alpha^j)^\dagger \psi + \psi^\dagger \alpha^j \frac{\partial \psi}{\partial x^j} \right) - \frac{imc}{\hbar}(\psi^\dagger \beta \psi - \psi^\dagger \beta^\dagger \psi). \tag{4.4}$$

We would like to write this as the divergence of something. That means, every term on the right hand side must contain a spatial derivative. Thus, the last term must vanish. This leads to the condition

$$\beta^\dagger = \beta, \tag{4.5}$$

i.e., β must be a Hermitian matrix. Then the remaining terms

$$-\sum_{j=1}^{3} \left(\frac{\partial \psi^\dagger}{\partial x^j}(\alpha^j)^\dagger \psi + \psi^\dagger \alpha^j \frac{\partial \psi}{\partial x^j} \right) \tag{4.6}$$

can be written as the divergence

$$-\sum_{j=1}^{3} \partial_j (\psi^\dagger \alpha^j \psi) \tag{4.7}$$

if we also have

$$(\alpha^j)^* = \alpha^j, \quad j = 1, 2, 3. \tag{4.8}$$

Thus, we obtain the *conserved 4-current*

$$j = (\psi^\dagger \psi, c\psi^\dagger \boldsymbol{\alpha} \psi) \tag{4.9}$$

where $\boldsymbol{\alpha} = (\alpha^1, \alpha^2, \alpha^3)$ is the 3-vector of α-matrices.

Now we have see what the second requirement amounts to. To this end, we let the operator

$$\frac{1}{c}\frac{\partial}{\partial t} - \sum_{j=1}^{3} \alpha^j \frac{\partial}{\partial x^j} - \frac{imc}{\hbar}\beta \tag{4.10}$$

act on (4.2). The idea behind this is to get second order derivatives into the equation which can then be compared with the KG equation. It is also somewhat analogous to decomposing a second order differential operator into a product of first order differential operators, such as the wave operator for 1+1 dimensions: $\partial_t^2 - \partial_x^2 = (\partial_t - \partial_x)(\partial_t + \partial_x)$. Here we get

$$\frac{1}{c^2}\frac{\partial^2 \psi}{\partial t^2} = \sum_{j,k=1}^{3} \frac{1}{2}(\alpha^j \alpha^k + \alpha^k \alpha^j) \frac{\partial^2 \psi}{\partial x^j \partial x^k} - \frac{m^2 c^2}{\hbar^2}\beta^2 \psi + \frac{imc}{\hbar} \sum_{j=1}^{3} (\alpha^j \beta + \beta \alpha^j) \frac{\partial \psi}{\partial x^j}. \tag{4.11}$$

In the first term of the r.h.s., we have used the symmetric rewriting $\sum_{j,k=1}^{3} \alpha^j \alpha^k \frac{\partial^2 \psi}{\partial x^j \partial x^k} = \sum_{j,k=1}^{3} \frac{1}{2}(\alpha^j \alpha^k + \alpha^k \alpha^j) \frac{\partial^2 \psi}{\partial x^j \partial x^k}$ which is possible for every $\psi \in C^2$.

At this point, we can clearly see which conditions requirement 2 implies. The r.h.s. of (4.11) reduces to $\nabla^2 \psi - \frac{m^2 c^2}{\hbar} \psi$ for all $\psi \in C^2$ if and only if for all $j, k = 1, 2, 3$:

$$\begin{cases} \frac{1}{2}(\alpha^j \alpha^k + \alpha^k \alpha^j) = \delta^{jk} \mathbb{1} \\ \alpha^k \beta + \beta \alpha^k = 0 \\ (\alpha^j)^2 = \mathbb{1} = \beta^2 \end{cases} \tag{4.12}$$

Here, δ^{jk} is the Kronecker delta.

Concrete realizations of the α and β matrices. We know already that α^j, $j = 1, 2, 3$ and β must be Hermitian. The next question is what their size K can be.

Lemma 4.1.1 (4.12) *implies that the size K of the α, β-matrices must be even.*

Proof: We write the second equation of (4.12) as

$$\beta \alpha^j = -\alpha^j \beta = (-\mathbb{1}) \alpha^j \beta \tag{4.13}$$

Taking the determinant yields:

$$\det \beta \det \alpha^j = (-1)^K \det \alpha^j \det \beta, \tag{4.14}$$

as $\det(-\mathbb{1}) = (-1)^K$. Thus, $(-1)^K = 1$ which implies that K is even. □

We know already that the minimum dimension of the α, β-matrices is 2×2. Furthermore, we have:

Lemma 4.1.2

$$\operatorname{tr} \alpha^j = 0 = \operatorname{tr} \beta, \quad j = 1, 2, 3. \tag{4.15}$$

Proof: Since β is Hermitian, we can diagonalize it. We choose a basis for which

$$\beta = \operatorname{diag}(b_1, ..., b_K). \tag{4.16}$$

Then, from $\beta^2 = \mathbb{1}$, we can conclude $b_i = \pm 1$, $i = 1, ..., K$. Moreover, from $\beta^2 = \mathbb{1} = (\alpha^j)^2$, each of these matrices is invertible. We can thus rewrite $\beta \alpha^j = -\alpha^j \beta$ as

$$(\alpha^j)^{-1} \beta \alpha^j = -\beta. \tag{4.17}$$

Now we take the trace of this equation and use the property $\operatorname{tr}(AB) = \operatorname{tr}(BA)$. This yields:

$$\operatorname{tr}[(\alpha^j)^{-1} \beta \alpha^j] = \operatorname{tr}(-\beta) \quad \Leftrightarrow \quad \operatorname{tr}[\alpha^j (\alpha^j)^{-1} \beta] = -\operatorname{tr} \beta \quad \Leftrightarrow \quad \operatorname{tr} \beta = -\operatorname{tr} \beta, \tag{4.18}$$

and hence $\operatorname{tr} \beta = 0$. As α^j is also Hermitian and $(\alpha^j)^2 = \mathbb{1}$ one can similarly show $\operatorname{tr} \alpha^j = 0$, $j = 1, 2, 3$. □

Lemma 4.1.3 *The minimum size of the α, β-matrices such that* (4.12) *can be satisfied is $K = 4$.*

Proof: We first show that $K = 2$ (which is the lowest even natural number) is not compatible with the properties (4.12). To this end, note that $\alpha^j,\ j = 1, 2, 3$ and β all have to be linearly independent. If this were not the case then one could write

$$\beta = \sum_{j=1}^{3} c_j \alpha^j, \quad c_j \in \mathbb{C},\ j = 1, 2, 3. \tag{4.19}$$

Multiplying this equation with α^l from the right for some $l \in \{1, 2, 3\}$ yields:

$$\beta\alpha^l = c_l(\alpha^l)^2 + \sum_{j=1, j\neq l}^{3} c_j \alpha^j \alpha^l. \tag{4.20}$$

On the other hand, as $\beta\alpha^l = -\alpha^l\beta$, we find:

$$\beta\alpha^l = -c_l(\alpha^l)^2 - \sum_{j=1, j\neq l}^{3} c_j \alpha^l \alpha^j. \tag{4.21}$$

Comparing the two expressions and using $\alpha^l\alpha^j = -\alpha^j\alpha^l$ as well as $(\alpha^l)^2 = \mathbb{1}$ yields: $c_l = 0$. Repeating the argument for all $l = 1, 2, 3$ yields $\beta = 0$ in contradiction with $\beta^2 = \mathbb{1}$. So all the matrices α^j, β must be linearly independent. However, it is a well-known fact that there are only three linearly independent anti-commuting 2×2 matrices. So $K > 2$.

The next greatest even number is $K = 4$. Indeed, for $K = 4$, it is possible to find Hermitian matrices α^j, β which satisfy all the requirements (4.12). Let

$$\sigma^1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma^2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma^3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \tag{4.22}$$

denote the Pauli matrices. Then one can easily check (**Sheet 6, Exercise 1**) that

$$\beta = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}, \quad \alpha^j = \begin{pmatrix} 0 & \sigma^j \\ \sigma^j & 0 \end{pmatrix} \tag{4.23}$$

are Hermitian and satisfy (4.12). □

Remarks.

- In lower spacetime dimensions, such as $d = 1, 2$, one needs fewer α-matrices (only d) and then it becomes possible to find 2×2 representations of the algebraic relations (4.12). → **Sheet 6, Exercise 1**.
- It is possible to find representations of the relations (4.12) for all $K = 4n$, $n \in \mathbb{N}$ (see e.g. Schweber p. 71) but these representations are reducible to the 4×4 representations. (That means, they can be brought into a block diagonal form with the 4×4 matrices on the diagonal.)

One should note that the matrices β, α^j are not unique. There are many different representations which are, however, equivalent in the following sense.

Lemma 4.1.4 *Let β, α^j as well as $\widetilde{\beta}, \widetilde{\alpha}^j$ ($j = 1, 2, 3$) be two sets of $K \times K$ matrices satisfying* (4.12). *Then there is an invertible matrix S such that*

$$\widetilde{\beta} = S\beta S^{-1}, \quad \widetilde{\alpha}^j = S\alpha^j S^{-1}, \quad j = 1, 2, 3. \tag{4.24}$$

The proof can, e.g., be found in Schweber p. 72.

4.2 Relativistic invariance of the Dirac equation

Invariant form and γ-matrices. Eq. (4.2) is not written in a manifestly Lorentz invariant form because of the splitting between time and spatial derivatives. Moreover, the term with the time derivatives does not contain any matrices in front. We shall now rewrite (4.2) in a form where Lorentz invariance is easier to see. We begin with multiplying (4.2) with $i\beta$ from the left. This yields (using $\beta^2 = \mathbb{1}$):

$$i\beta\frac{1}{c}\frac{\partial\psi}{\partial t} + i\sum_{j=1}^{3}\beta\alpha^j\frac{\partial\psi}{\partial x^j} - \frac{mc}{\hbar}\psi = 0. \tag{4.25}$$

Now we introduce a new set of matrices $\gamma^\mu,\ \mu = 0,1,2,3$ (which is equivalent to specifying β and $\alpha^j,\ j = 1,2,3$):

$$\gamma^0 = \beta, \quad \gamma^j = \beta\alpha^j,\ j = 1,2,3. \tag{4.26}$$

Explicitly, the previous representation of the α,β-matrices leads to:

$$\gamma^0 = \begin{pmatrix} \mathbb{1}_2 & 0 \\ 0 & -\mathbb{1}_2 \end{pmatrix}, \quad \gamma^j = \begin{pmatrix} 0 & \sigma^j \\ -\sigma^j & 0 \end{pmatrix},\ j = 1,2,3. \tag{4.27}$$

Using summation convention and setting $c = 1 = \hbar$, (4.25) can be rewritten very concisely as:

$$(i\gamma^\mu\partial_\mu - m)\psi(x) = 0. \tag{4.28}$$

This will be the form of the Dirac equation we shall be using most in this class.

To rewrite the 4-current $j = (\psi^\dagger\psi, c\psi^\dagger\alpha\psi)$ in terms of γ-matrices, we introduce the *Dirac conjugate* $\overline{\psi}$ of ψ:

$$\overline{\psi} = \psi^\dagger\gamma^0. \tag{4.29}$$

Then noting that $(\gamma^0)^2 = \beta^2 = \mathbb{1}$, we have:

$$j^\mu = \overline{\psi}\gamma^\mu\psi. \tag{4.30}$$

The anti-commutation relation of the α,β-matrices (4.12) translate to the following anti-commutation relations for the γ-matrices:

$$\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu}\,\mathbb{1}. \tag{4.31}$$

These relations are called *Clifford algebra relations.*You should always try to reduce all calculations with γ-matrices to these relations. This is *much* simpler than the explicit matrix representation above. In fact, one can almost forget that the γ^μ are matrices. Here is a demonstration. We show again that every component of the Dirac equation satisfies the KG equation. We act on (4.28) with the operator $-(i\gamma^\nu\partial_\nu + m)$. This leads to:

$$\begin{aligned} & -(i\gamma^\nu\partial_\nu + m)(i\gamma^\mu\partial_\mu - m)\psi = 0 \\ \Leftrightarrow\quad & (\gamma^\mu\gamma^\nu\partial_\mu\partial_\nu + i\gamma^\nu m - i\gamma^\mu m + m^2)\psi = 0 \\ \Leftrightarrow\quad & (\tfrac{1}{2}(\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu)\partial_\mu\partial_\nu + m^2)\psi = 0 \\ \Leftrightarrow\quad & (\eta^{\mu\nu}\partial_\mu\partial_\nu + m^2)\psi = 0 \\ \Leftrightarrow\quad & (\partial_\mu\partial^\mu + m^2)\psi = 0. \end{aligned} \tag{4.32}$$

This is the KG equation (satisfied by each component of ψ).

It is, moreover, useful to note the following relations for the Hermitian conjugate of γ^μ:

$$(\gamma^0)^\dagger = \gamma^0, \quad (\gamma^j)^\dagger = -\gamma^j, \ j = 1, 2, 3. \tag{4.33}$$

The first relation results from $(\gamma^0)^\dagger = \beta^\dagger = \beta$ and the second from $(\gamma^j)^\dagger = (\beta\alpha^j)^\dagger = (\alpha^j)^\dagger\beta^\dagger = \alpha^j\beta = -\beta\alpha^j = -\gamma^j$. One can avoid the case differentiation in (4.33) by rewriting (4.33) equivalently as

$$(\gamma^\mu)^\dagger = \gamma^0\gamma^\mu\gamma^0. \tag{4.34}$$

Remark. The relation of Eq. (4.31) to the theory of Clifford algebras can be seen as follows.

Definition: (i) Let V be an n-dimensional vector space ($n \in \mathbb{N}$) over a field $\mathbb{K}$ and $Q : V \to \mathbb{K}$ be a quadratic form on V. Then the *Clifford algebra* $Cl(V, Q)$ is defined as the algebra over $\mathbb{K}$ which is generated by V and the unit element $\mathbb{1}_{Cl}$, and whose multiplication relation satisfies

$$v \cdot v = -Q(v)\,\mathbb{1}_{Cl} \quad \forall v \in V. \tag{4.35}$$

(ii) Let now $V = \mathbb{R}^n$, $\mathbb{K} = \mathbb{R}$ and $p, q \in \mathbb{N}_0$ such that $p + q = n$. For $x \in \mathbb{R}^n$, we then let

$$Q(x) = -(x^0)^2 - \cdots - (x^{p-1})^2 + (x^p)^2 + \cdots + (x^{n-1})^2 \tag{4.36}$$

and denote the real Clifford algebra $Cl(\mathbb{R}^n, Q)$ (according to (i)) by $Cl(p, q, \mathbb{R})$.

Why does Eq. (4.31) relate to the definition of a Clifford algebra? To see this, we define, for all $x \in \mathbb{R}^4$:

$$\gamma(x) = \gamma_\mu x^\mu. \tag{4.37}$$

Furthermore, we let

$$Q(x) = -x^\mu x_\mu = -(x^0)^2 + (x^1)^2 + (x^2)^2 + (x^3)^2. \tag{4.38}$$

Then $Cl(1, 3, \mathbb{R})$ is given by the set

$$Cl(1, 3, \mathbb{R}) = \{\gamma(x) : x \in \mathbb{R}^4\} \tag{4.39}$$

together with the addition and multiplication of matrices as the algebra relations. The Clifford algebra relation (4.35) is then equivalent to:

$$\begin{aligned}
& \gamma(x) \cdot \gamma(x) = x_\mu x^\mu\, \mathbb{1} \ \ \forall x \in \mathbb{R}^4 \\
\Leftrightarrow \quad & (x_\mu\gamma^\mu)(x_\nu\gamma^\nu) = x_\mu x^\mu\, \mathbb{1} \ \ \forall x \in \mathbb{R}^4 \\
\Leftrightarrow \quad & \frac{1}{2}x_\mu x_\nu(\gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu) = x_\mu x_\nu\, \eta^{\mu\nu}\, \mathbb{1} \ \ \forall x \in \mathbb{R}^4 \\
\Leftrightarrow \quad & \gamma^\mu\gamma^\nu + \gamma^\nu\gamma^\mu = 2\eta^{\mu\nu}\, \mathbb{1}.
\end{aligned} \tag{4.40}$$

This is exactly Eq. (4.31).

Transformation law for the Dirac equation. We already know from the discussion of the Salpeter equation that $\rho = |\psi|^2$ (and, for that matter, also $\rho = \psi^\dagger\psi$) will transform as a scalar if ψ transforms as a scalar. So in order for $j^\mu = (\psi^\dagger\psi, \overline{\psi}\gamma^j\psi)$ to transform as a vector, we need a different transformation law for ψ. The vector structure of the wave function in the Dirac equation gives us the flexibility to implement more general transformation laws. We shall try to use following transformation law under Poincaré transformations (a, Λ):

$$\psi'(x') = S[\Lambda]\psi(x) \quad \Leftrightarrow \quad \psi'(x') = S[\Lambda]\psi(\Lambda^{-1}(x'-a)), \tag{4.41}$$

where $S[\Lambda]$ is an invertible complex 4×4 matrix determined by Λ. (We shall say more about its exact definition and its relation to a representation of the Poincaré group later.)

We now determine the conditions for $S[\Lambda]$ such that the Dirac equation is invariant under Poincaré transformations and the law (4.41). That means, if $\psi(x)$ satisfies $(i\gamma^\mu\partial_\mu - m)\psi(x) = 0$, we want that $\psi'(x')$ satisfies $(i\gamma^\mu\partial'_\mu - m)\psi'(x') = 0$.

We start with the Dirac equation for $\psi(x)$. Then we use (4.41) to express $\psi(x)$ in terms of $\psi'(x')$, i.e.:

$$(i\gamma^\mu\partial_\mu - m)S[\Lambda]^{-1}\psi'(x') = 0 \tag{4.42}$$

Now we have the following transformation rule for the derivatives:

$$\frac{\partial}{\partial x^\mu} = \frac{\partial x'^\nu}{\partial x^\mu}\frac{\partial}{\partial x'^\nu} = \Lambda^\nu{}_\mu\,\partial'_\nu. \tag{4.43}$$

Using this in (4.42) yields:

$$(i\gamma^\mu\Lambda^\nu{}_\mu\,\partial'_\nu - m)S[\Lambda]^{-1}\psi'(x') = 0. \tag{4.44}$$

We now multiply with $S[\Lambda]$.This yields:

$$(iS[\Lambda]\gamma^\mu S[\Lambda]^{-1}\Lambda^\nu{}_\mu\,\partial'_\nu - m)\psi'(x') = 0. \tag{4.45}$$

From this expression we read off that we need

$$S[\Lambda]\gamma^\mu\Lambda^\nu{}_\mu S[\Lambda]^{-1} = \gamma^\nu \tag{4.46}$$

or, equivalently

$$S[\Lambda]^{-1}\gamma^\nu S[\Lambda] = \Lambda^\nu{}_\mu\gamma^\mu. \tag{4.47}$$

This will be the main requirement for the matrices $S[\Lambda]$.

Construction of the matrices $S[\Lambda]$.

Lemma 4.2.1 *Let $\Lambda \in \mathcal{L}_+^\uparrow$. Then:*

(a) There exists a complex 4×4 matrix $S[\Lambda]$ such that (4.47) holds.

(b) Let $S_1[\Lambda]$ and $S_2[\Lambda]$ be two complex 4×4 matrices satisfying (4.47). Then there is a $c \in \mathbb{C}\backslash\{0\}$ such that $S_2[\Lambda] = c\,S_1[\Lambda]$.

Proof: (a) Let $\gamma'^{\nu} = \Lambda^{\nu}{}_{\mu}\gamma^{\mu}$, $\nu = 0, 1, 2, 3$. Then it is easy to verify using (4.47) that we have:

$$\gamma'^{\mu}\gamma'^{\nu} + \gamma'^{\nu}\gamma'^{\mu} = 2\eta^{\mu\nu}\,\mathbb{1}. \tag{4.48}$$

We now know from before that then there exists an invertible matrix S such that $S^{-1}\gamma^{\mu}S = \gamma'^{\mu}\ \forall\mu$.

(b) We then have: $S_1[\Lambda]^{-1}\gamma^{\mu}S_1[\Lambda] = \Lambda^{\mu}{}_{\nu}\gamma^{\nu} = S_2[\Lambda]^{-1}\gamma^{\mu}S_2[\Lambda]$. Multiplying this relation with $S_2[\Lambda]$ from the left and $S_1[\Lambda]^{-1}$ from the right yields:

$$S_2[\Lambda]S_1[\Lambda]^{-1}\gamma^{\mu} = \gamma^{\mu}S_2[\Lambda]S_1[\Lambda]^{-1}\ \ \forall\mu. \tag{4.49}$$

Thus, the matrix $S_2[\Lambda]S_1[\Lambda]^{-1}$ commutes with all γ-matrices and is therefore (as a basis of $\mathbb{C}^{4\times4}$ can be constructed from products of γ-matrices, see e.g. Schweber p. 71) proportional to the identity matrix, i.e. there is a $c \in \mathbb{C}\backslash\{0\}$ such that $S_2[\Lambda]S_1[\Lambda]^{-1} = c\,\mathbb{1}$. This is yields the claim. □

Next, we determine the Hermitian conjugate of $S[\Lambda]$. Among other things, we need this to determine $\overline{\psi}' = \psi'^{\dagger}\gamma^0$.

Lemma 4.2.2 *Let $\Lambda \in \mathcal{L}_+^{\uparrow}$ and let $S[\Lambda]$ be a complex 4×4 matrix which satisfies* (4.47)*. Furthermore, choose a normalization such that* $\det S[\Lambda] = 1$*. Then:*

$$S[\Lambda]^{\dagger} = \gamma^0 S[\Lambda]^{-1}\gamma^0. \tag{4.50}$$

Proof: In the proof we abbreviate $S[\Lambda] =: S$. We first show that there is a number $b \in \mathbb{R}$ such that $S^{\dagger}\gamma^0 = b\gamma^0 S^{-1}$. To this end, we take the Hermitian conjugate of (4.47) and multiply with γ^0 from both sides. This yields:

$$\gamma^0\Lambda^{\nu}{}_{\mu}(\gamma^{\mu})^{\dagger}\gamma^0 = \gamma^0(S^{-1}\gamma^{\nu}S)^{\dagger}\gamma^0 \tag{4.51}$$

Now we use the identity $(\gamma^{\mu})^{\dagger} = \gamma^0\gamma^{\mu}\gamma^0$. This yields:

$$\Lambda^{\nu}{}_{\mu}\gamma^{\mu} = (\gamma^0 S^{\dagger}\gamma^0)\gamma^{\nu}(\gamma^0 S^{\dagger}\gamma^0)^{-1}, \tag{4.52}$$

where we also used $(\gamma^0)^{-1} = \gamma^0$. Now we identify the left hand side with $S^{-1}\gamma^{\nu}S$. This yields:

$$\begin{aligned} & S^{-1}\gamma^{\nu}S = (\gamma^0 S^{\dagger}\gamma^0)\gamma^{\nu}(\gamma^0 S^{\dagger}\gamma^0)^{-1} \\ \Leftrightarrow\quad & \gamma^{\nu}\,(S\gamma^0 S^{\dagger}\gamma^0) = (S\gamma^0 S^{\dagger}\gamma^0)\gamma^{\nu}. \end{aligned} \tag{4.53}$$

So we have found that $S\gamma^0 S^{\dagger}\gamma^0$ commutes with all the gamma matrices. Hence it is proportional to the identity, i.e., there is a $b \in \mathbb{C}\backslash\{0\}$ such that

$$S\gamma^0 S^{\dagger}\gamma^0 = b\,\mathbb{1}. \tag{4.54}$$

This is equivalent to

$$S\gamma^0 S^{\dagger} = b\gamma^0. \tag{4.55}$$

Now the left hand side is Hermitian by its very form and $(\gamma^0)^{\dagger} = \gamma^0$. Thus we must also have $b \in \mathbb{R}$.

Next, we show that $b = 1$. We take the determinant of (4.54) and use $\det S = 1$. This yields: $b^4 = 1$, hence $b \in \{-1, +1\}$. To show that $b = +1$, we $S^\dagger S$ using that

$$S^\dagger = b\,\gamma^0 S^{-1}\gamma^0 \tag{4.56}$$

by virtue of (4.55).

$$\begin{aligned} S^\dagger S &= b\gamma^0 S^{-1}\gamma^0 S \\ &= b\gamma^0 \Lambda^0{}_\mu \gamma^\mu = b\left(\Lambda^0{}_0\,\mathbb{1} + \Lambda^0{}_j \gamma^0\gamma^j\right). \end{aligned} \tag{4.57}$$

Now we take the trace using that $\operatorname{tr}(\gamma^0\gamma^j) = \operatorname{tr}\alpha^j = 0$ and obtain:

$$\operatorname{tr}(S^\dagger S) = 4b\Lambda^0{}_0. \tag{4.58}$$

Next, note that the matrix $S^\dagger S$ is Hermitian and positive definite by its very form (it is non-negative as S is invertible). Thus, all of its eigenvalues are real and positive. Hence $\operatorname{tr}(S^\dagger S) > 0$. As we also have $\Lambda^0{}_0 > 0$ for $\Lambda \in \mathcal{L}_+^\uparrow$, it follows that $b > 0$, so $b = +1$. Then (4.56) yields the claim. □

Next, we construct the possible matrices $S[\Lambda]$ explicitly for $\Lambda \in \mathcal{L}_+^\uparrow$.

Theorem 4.2.3 *Let $\Lambda \in \mathcal{L}_+^\uparrow$. Let $M^{\mu\nu} = -M^{\nu\mu}$, $\mu, \nu = 0, 1, 2, 3$ be the generators of the Lorentz Lie algebra, i.e. the 4×4 matrices with elements*

$$(M^{\mu\nu})^{\rho\sigma} = \eta^{\rho\mu}\eta^{\sigma\nu} - \eta^{\sigma\mu}\eta^{\rho\nu} \tag{4.59}$$

and $\omega_{\mu\nu} = -\omega_{\nu\mu}$ be those real number such that $\Lambda = \exp(\omega_{\mu\nu}M^{\mu\nu}/2)$ (see Eq. (2.26)). Then a matrix satisfying Eq. (4.47) is given by:

$$S[\Lambda] = \exp(\omega_{\mu\nu}S^{\mu\nu}/2). \tag{4.60}$$

where

$$S^{\mu\nu} = \frac{1}{4}[\gamma^\mu, \gamma^\nu], \quad \mu, \nu = 0, 1, 2, 3. \tag{4.61}$$

Proof: We show the claim for an infinitesimal Lorentz transformation

$$\Lambda = \mathbb{1} + \frac{1}{2}\omega_{\mu\nu}M^{\mu\nu}, \tag{4.62}$$

where $\omega_{\mu\nu}$ are infinitesimally small parameters. The statement for a finite Lorentz transformation can then be obtained by exponentiation.
Up to first order in the parameters $\omega_{\mu\nu}$, we then have:

$$\Lambda^\mu{}_\nu = \delta^\mu_\nu + \frac{1}{2}\omega_{\rho\sigma}(M^{\rho\sigma})^\mu{}_\nu \tag{4.63}$$

as well as

$$S[\Lambda] = \mathbb{1} + \frac{1}{2}\omega_{\rho\sigma}S^{\rho\sigma}. \tag{4.64}$$

Furthermore, (4.47) amounts to:

$$(\mathbb{1} - \tfrac{1}{2}\omega_{\rho\sigma}S^{\rho\sigma})\gamma^\mu(\mathbb{1} + \tfrac{1}{2}\omega_{\alpha\beta}S^{\alpha\beta}) = (\delta^\mu_\nu + \tfrac{1}{2}\omega_{\rho\sigma}(M^{\rho\sigma})^\mu{}_\nu)\gamma^\nu. \tag{4.65}$$

Up to first order in $\omega_{\mu\nu}$, this is equivalent to:

$$\begin{aligned} & \gamma^\mu - \tfrac{1}{2}\omega_{\rho\sigma} S^{\rho\sigma}\gamma^\mu + \tfrac{1}{2}\gamma^\mu \omega_{\rho\sigma} S^{\rho\sigma} = \gamma^\mu + \tfrac{1}{2}\omega_{\rho\sigma}(M^{\rho\sigma})^\mu{}_\nu \gamma^\nu \\ \Leftrightarrow \quad & [\gamma^\mu, S^{\rho\sigma}] = (M^{\rho\sigma})^\mu{}_\nu \gamma^\nu. \end{aligned} \tag{4.66}$$

In order to prove this matrix equation, we first note that according to (4.59)

$$(M^{\rho\sigma})^\mu{}_\nu = \eta^{\rho\mu}\delta^\sigma_\nu - \eta^{\sigma\mu}\delta^\rho_\nu \tag{4.67}$$

so that

$$(M^{\rho\sigma})^\mu{}_\nu \gamma^\nu = \eta^{\rho\mu}\gamma^\sigma - \eta^{\sigma\mu}\gamma^\rho. \tag{4.68}$$

Next, note that $S^{\rho\sigma} = 0$ for $\rho = \sigma$ and $S^{\rho\sigma} = \frac{1}{2}\gamma^\rho\gamma^\sigma$. This can be summarized as

$$S^{\rho\sigma} = \tfrac{1}{2}\gamma^\rho\gamma^\sigma - \tfrac{1}{2}\eta^{\rho\sigma}\,\mathbb{1}. \tag{4.69}$$

Using this identity, we obtain:

$$\begin{aligned} [\gamma^\mu, S^{\rho\sigma}] &= \tfrac{1}{2}\gamma^\mu\gamma^\rho\gamma^\sigma - \gamma^\rho\gamma^\sigma\gamma^\mu \\ &= \tfrac{1}{2}\{\gamma^\mu, \gamma^\rho\}\gamma^\sigma - \tfrac{1}{2}\gamma^\rho\gamma^\mu\gamma^\sigma - \tfrac{1}{2}\gamma^\rho\{\gamma^\sigma, \gamma^\mu\} + \tfrac{1}{2}\gamma^\rho\gamma^\mu\gamma^\sigma \\ &= \eta^{\mu\rho}\gamma^\sigma - \eta^{\sigma\mu}\gamma^\rho. \end{aligned} \tag{4.70}$$

Comparing this with (4.68), we indeed obtain the same result (note $\eta^{\mu\rho} = \eta^{\rho\mu}$). Thus (4.66) is indeed satisfied and the claim follows. □

Ambiguity of the matrices $S[\Lambda]$. We now ask if the matrices $S[\Lambda]$ are determined uniquely by $\Lambda \in \mathcal{L}^\uparrow_+$. To this end, consider the matrix $S[\Lambda]$ for a rotation $\Lambda = R_1(\theta)$ around the x^1 axis by an angle θ, i.e.

$$R_1 = \exp(\theta M^{23}). \tag{4.71}$$

We then have according to (4.60): ($\omega_{23} = -\omega_{32} = \theta$ and all other coefficients $\omega_{\mu\nu} = 0$):

$$S[R_1] = \exp(\theta S^{23}) = \exp(\tfrac{\theta}{4}(\gamma^2\gamma^3 - \gamma^3\gamma^2)) = \exp(\tfrac{\theta}{2}\gamma^2\gamma^3). \tag{4.72}$$

Now, in our representation,

$$\gamma^2\gamma^3 = \begin{pmatrix} -i\sigma^1 & 0 \\ 0 & -i\sigma^1 \end{pmatrix}. \tag{4.73}$$

Thus, considering $(\sigma^1)^{2k} = \mathbb{1}_2$ and $(\sigma^1)^{2k-1} = \sigma^1$ for $k \in \mathbb{N}$, we find:

$$\begin{aligned} S[R_1(\theta)] &= \sum_{k=1}^{\infty} \frac{(\theta/2)^k(-i)^k}{k!} \begin{pmatrix} (\sigma^1)^k & 0 \\ 0 & (\sigma^1)^k \end{pmatrix} \\ &= \cos(\tfrac{\theta}{2})\,\mathbb{1}_4 - i\sin(\tfrac{\theta}{2}) \begin{pmatrix} \sigma^1 & 0 \\ 0 & \sigma^1 \end{pmatrix}. \end{aligned} \tag{4.74}$$

Therefore, we arrive at the surprising fact that

$$S[R_1(\theta + 2\pi)] = -S[R_1(\theta)]. \tag{4.75}$$

As $R_1(\theta + 2\pi) = R_1(\theta)$, this means that there are two matrices $S[R_1(\theta)]$, differing in their sign. This is the case for every rotation.

For boosts, this phenomenon does not occur. For example, for a boost Λ in x^1-direction and with boost parameter ω, we have:

$$S[\Lambda] = \exp(\tfrac{\omega}{2}\gamma^0\gamma^1). \tag{4.76}$$

Noting $(\gamma^0\gamma^1)^2 = (\alpha^1)^2 = \mathbb{1}_4$, we obtain:

$$S[\Lambda] = \cosh(\tfrac{\omega}{2})\mathbb{1}_4 + \alpha^1 \sinh(\tfrac{\omega}{2}). \tag{4.77}$$

This is in injective function of ω. Thus, there is only one matrix $S[\Lambda]$ for the boost Λ.

Relation of the transformation law to representations of the Poincaré group. The fact that there may be an ambiguity in sign of the matrices $S[\Lambda]$ means that the map $\rho : \mathcal{L}_+^\uparrow \to \mathbb{C}^{4\times 4}$, $\Lambda \mapsto S[\Lambda]$ is not a representation in the usual sense. However, it is still related to a different kind of representation. One should realize that the phase of a Dirac wave function ψ is physically irrelevant, as all physical properties are based on bilinear quantities such as the current $j^\mu = \overline{\psi}\gamma^\mu\psi$ which do not depend on this phase. One therefore often identifies wave function differing only by a phase (or, in fact, even by normalization):

$$\psi \sim \psi' \quad :\Leftrightarrow \quad \exists \lambda \in \mathbb{C}\backslash\{0\} : \psi = \lambda\psi'. \tag{4.78}$$

The space of such equivalence classes of wave functions (the initial space for example being the Hilbert space $L^2(\mathbb{R}^3, \mathbb{C}^4)$) is a projective space. Then an ambiguity of phases in the representation does not matter, and the matrices $S[\Lambda]$ define a so-called *projective representation* of the (proper) Lorentz group on that space. See the book by Thaller for extensive details.[2]

Transformation laws of quantities involving $\psi, \overline{\psi}$ and γ-matrices. As a consequence of the transformation behavior (4.47), one readily obtains the following theorem (→ **Sheet 7, Exercise 1**).

Theorem 4.2.4 *Let $\psi : \mathbb{R}^4 \to \mathbb{C}^4$ transform under Poincaré transformations (a, Λ) as in* (4.41) *with $S[\Lambda]$ given by* any *of the two possible matrices. Then*

$$S(x) = \overline{\psi}(x)\psi(x), \quad j^\mu(x) = \overline{\psi}(x)\gamma^\mu\psi(x), \quad T^{\mu\nu}(x) = \overline{\psi}(x)\gamma^\mu\gamma^\nu\psi(x), \quad \textit{etc.} \tag{4.79}$$

transform as

$$S'(x') = S(x), \quad j'^\mu(x') = \Lambda^\mu{}_\nu j^\nu(x), \quad T'^{\mu\nu}(x') = \Lambda^\mu{}_\rho\Lambda^\nu{}_\sigma T^{\rho\sigma}(x), \quad \textit{etc.} \tag{4.80}$$

In particular, this means that j transforms in the right way under (proper) Lorentz transformations. Note that the possible ambiguity in the sign of the matrices $S[\Lambda]$ does not affect the above transformation behavior as $S[\Lambda]$ occurs both in ψ and $\overline{\psi}$, and a possible phase thus cancels.

[2] B. Thaller: *The Dirac Equation*, Springer 1992, Chap. 2.

4.3 Discrete Transformations.

In order to obtain the transformation behavior under the full Lorentz group, we need to know how ψ transforms under space and time reflections. We shall be brief here and only state the transformation behavior without giving a derivation.

Space-reflection (parity). For a space reflection $\mathbf{P} : x = (t, \mathbf{x}) \mapsto x' = (t, -\mathbf{x})$, we postulate the transformation behavior

$$\psi'(x') = \gamma^0 \psi(x) \tag{4.81}$$

or equivalently

$$\psi'(t, \mathbf{x}) = \gamma^0 \psi(t, -\mathbf{x}). \tag{4.82}$$

Now it follows that $\psi'(x')$ satisfies the Dirac equation in the primed variables if $\psi(x)$ solves the Dirac equation in the unprimed variables $\rightarrow$ **Sheet 8, Exercise 1**.

Time-reflection. For a time reflection $\mathbf{T} : x = (t, \mathbf{x}) \mapsto x' = (-t, \mathbf{x})$ we postulate the transformation behavior

$$\psi'(x') = B\psi^*(x) \tag{4.83}$$

or equivalently

$$\psi'(t, \mathbf{x}) = B\psi^*(-t, \mathbf{x}), \tag{4.84}$$

where $(\cdot)^*$ denotes complex conjugation and B is an invertible complex 4×4 matrix which needs to satisfy

$$B(\gamma^{0*}, -\boldsymbol{\gamma}^*)B^{-1} = (\gamma^0, \boldsymbol{\gamma}). \tag{4.85}$$

We may take

$$B = \gamma^1 \gamma^2, \tag{4.86}$$

for which $B^{-1} = -B$.

One can then show that the Dirac equation for $\psi(x)$ implies the Dirac equation for $\psi'(x') \rightarrow$ **Sheet 8, Exercise 1**.

Transformation behavior of bilinear quantities involving $\psi, \overline{\psi}$ under $\mathbf{P}, \mathbf{T}$:

Theorem 4.3.1 *Under* $\mathbf{P}$*, as well as under* $\mathbf{T}$ *we have* ($\delta_0^\mu = 1$ *if* $\mu = 0$ *and 0 else):*

$$\begin{aligned} \overline{\psi}'(x')\psi'(x') &= \overline{\psi}(x)\psi(x) \\ \overline{\psi}'(x')\gamma^\mu\psi'(x') &= (-1)^{1-\delta_0^\mu}\,\overline{\psi}(x)\gamma^\mu\psi(x) \\ \overline{\psi}'(x')\gamma^\mu\gamma^\nu\psi'(x') &= (-1)^{\delta_0^\mu+\delta_0^\nu}\,\overline{\psi}(x)\gamma^\mu\gamma^\nu\psi(x). \end{aligned} \tag{4.87}$$

The proof of the second equality will be carried out on **Sheet 8, Exercise 1**. The other ones follow similarly.

Charge conjugation. There is a further symmetry of the Dirac equation which we list here for completeness. It is, however, not a Poincaré transformation. We define a *charge-conjugated* wave function by

$$\psi'(x) = C\overline{\psi}(x)^T \tag{4.88}$$

where $(\cdot)^T$ denotes the transpose and C is an invertible complex 4×4 matrix which satisfies

$$C(\gamma^\mu)^T C^{-1} = -\gamma^\mu, \quad \mu = 0, 1, 2, 3. \tag{4.89}$$

One can, for example, use

$$C = i\gamma^0\gamma^2. \tag{4.90}$$

Then it can be shown that $\psi'(x)$ satisfies the Dirac equation if $\psi(x)$ does. However, as we shall come to now, one can show more, which also explains the name "charge conjugation".

Charge conjugation and the Dirac equation with an external field Assume a Dirac particle (electron) with charge $-e$ is placed in an external electromagnetic field described by a vector potential $A_\mu(x)$. Such a field gets implemented in the Dirac equation via *minimal coupling*, i.e. by replacing

$$i\partial_\mu \to i\partial_\mu - eA_\mu(x). \tag{4.91}$$

In this way, one obtains the Dirac equation with an external electromagnetic field:

$$[\gamma^\mu(i\partial_\mu - eA_\mu(x)) - m]\psi(x) = 0. \tag{4.92}$$

As a side remark, note that for a pure Coulomb field, $A_\mu(x) = (q/|\mathbf{x}|, 0, 0, 0)$, this equation is explicitly solvable. This yields an improved energy spectrum for the hydrogen atom (both the proton and the electron are spin-$\frac{1}{2}$ particles which can be described by the Dirac equation).

Lemma 4.3.2 *If $\psi(x)$ satisfies* (4.92)*, then the charge conjugated wave function $\psi'(x) = C\overline{\psi}^T(x)$ solves the same equation but with charge $+e$ instead of $-e$.*

Proof: Sheet 8, Exercise 1.

4.4 Physical properties

Properties of the probability current. In order for $j^\mu(x) = \overline{\psi}(x)\gamma^\mu\psi(x)$ to define a probability current density, the following properties are required:

1. $\partial_\mu j^\mu(x) = 0$ for solutions ψ of the Dirac equation,
2. j transforms under (proper) Poincaré transformations (a, Λ) as a vector field.
3. j is future-pointing and time-like.

We have already demonstrated properties 1. and 2., but 3. a demonstration of 3. is still lacking.

Lemma 4.4.1 *Let $\psi \in C^1(\mathbb{R}^4, \mathbb{C}^4)$ be a solution of the Dirac equation. Then the Dirac current $j^\mu(x) = \overline{\psi}(x)\gamma^\mu\psi(x)$ is future-pointing and time-like (or light-like).*

Proof: The claim is equivalent to $n_\mu j^\mu \geq 0$ for all time-like future-pointing unit vectors n. So pick such an n. Then there is a frame where $n' = (1, 0, 0, 0)$. In that frame:

$$n'_\mu j'^\mu = j'^0 = \psi'^\dagger \psi' \geq 0. \tag{4.93}$$

Let Λ be the Lorentz transformation which realizes $n'_\mu = (\Lambda^{-1})^\nu{}_\mu n_\nu$. As $n'_\mu j'^\mu = (\Lambda^{-1})^\nu{}_\mu \, n_\nu \, \Lambda^\mu{}_\sigma j^\sigma = n_\mu j^\mu$, (4.93) is indeed equivalent to $n_\mu j^\mu \geq 0$. □

The Dirac current thus satisfies all of our requirements! This makes an interpretation as a probability current possible. Among other things, we have:

Theorem 4.4.2 (Total probability conservation in all Lorentz frames.) *Let $\psi \in C^1(\mathbb{R}^4)$ be a solution of the Dirac equation and $\psi'(x') = S[\Lambda]\psi(x)$ as in (4.41). Then for all $t, t' \in \mathbb{R}$, we have:*

$$\int d^3\mathbf{x}\, \psi^\dagger(t, \mathbf{x})\psi(t, \mathbf{x}) = \int d^3\mathbf{x}'\, \psi'^\dagger(t', \mathbf{x}')\psi'(t', \mathbf{x}'). \tag{4.94}$$

Proof: Sheet 8, Exercise 2.

The most important consequence of 1.-3. is not this global statement but a local one: compatibility with the **Born rule**. First we give a statement referring to one particular frame, then one that is frame-independent:

Born rule, statement in one particular frame.

> $\psi^\dagger(t, \mathbf{x})\psi(t, \mathbf{x})d^3\mathbf{x}$ is the probability to find an electron in the infinitesimal volume $d^3\mathbf{x}$ around the location $\mathbf{x} \in \mathbb{R}^3$ at time t.

Born rule, frame-independent version.

> Let Σ be any (smooth) Cauchy surface and n its normal vector field. Then $n_\mu(x)\, \overline{\psi}(x)\gamma^\mu\psi(x)\, d\sigma(x)$ is the probability that the electron's world line crosses Σ in the infinitesimal 3-volume $d\sigma(x)$ around the spacetime point $x \in \mathbb{M}$.

Finite propagation speed.

Definition: We say that the Dirac equation has *finite propagation speed* if for all solutions $\psi \in C^1(\mathbb{R}^4)$ of the Dirac equation with $\operatorname{supp}\psi(0, \cdot) \subset B_r(0)$, one also has $\operatorname{supp}\psi(t, \cdot) \subset B_{r+t}(0)$ for all $t \geq 0$.

Theorem 4.4.3 *The Dirac equation has finite propagation speed.*

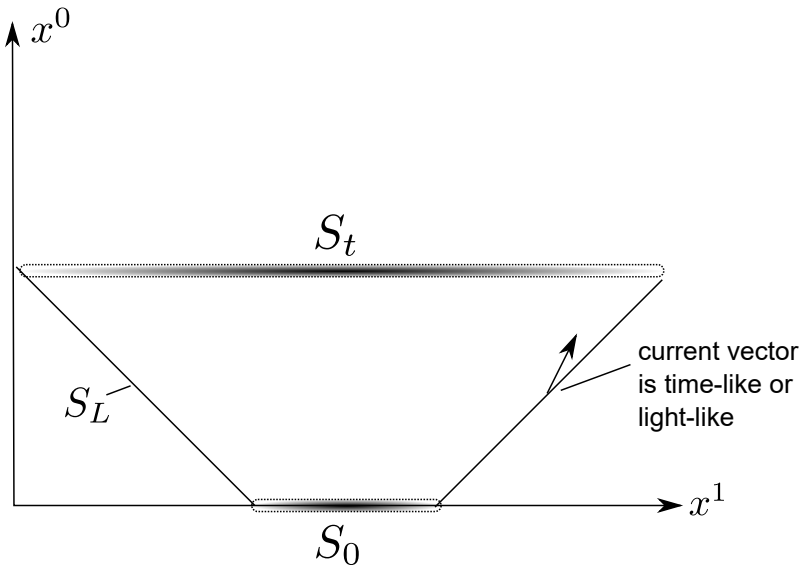

Figure 4.1: Illustration of the sets appearing in the proof of finite propagation speed.

Proof: Consider the closed surface (see also Fig. 4.1)

$$S = S_0 \cup S_t \cup S_L \tag{4.95}$$

with $S_0 = \{0\} \times B_r(0)$, $S_t = \{t\} \times B_{r+t}(0)$ and S_L being the light-like surface which makes S a closed surface.

Let ψ be a solution of the Dirac equation with $\operatorname{supp}\psi(0,\cdot) \subset B_r(0)$. Then the divergence theorem implies (considering what the exterior normal vectors are):

$$\begin{aligned} &\int_S d\sigma(x)\, n_\mu(x)\overline{\psi}(x)\gamma^\mu\psi(x) = 0 \\ \Leftrightarrow\quad &\int_{B_r(0)} d^3\mathbf{x}\,\psi^\dagger(0,\mathbf{x})\psi(0,\mathbf{x}) = \int_{B_{r+t}(0)} d^3\mathbf{x}\,\psi^\dagger(t,\mathbf{x})\psi(t,\mathbf{x}) - \int_{S_L} d\sigma(x)\, n_\mu(x)\overline{\psi}(x)\gamma^\mu\psi(x). \end{aligned} \tag{4.96}$$

On the other hand, total probability conservation yields:

$$\begin{aligned} &\int d^3\mathbf{x}\,\psi^\dagger(0,\mathbf{x})\psi(0,\mathbf{x}) = \int d^3\mathbf{x}\,\psi^\dagger(t,\mathbf{x})\psi(t,\mathbf{x}) \\ \Leftrightarrow\quad &\int_{B_r(0)} d^3\mathbf{x}\,\psi^\dagger(0,\mathbf{x})\psi(0,\mathbf{x}) = \int_{B_{r+t}(0)} d^3\mathbf{x}\,\psi^\dagger(t,\mathbf{x})\psi(t,\mathbf{x}) + \int_{\mathbb{R}^3\setminus B_{r+t}(0)} d^3\mathbf{x}\,\psi^\dagger(t,\mathbf{x})\psi(t,\mathbf{x}). \end{aligned} \tag{4.97}$$

Comparing this with (4.96), we find:

$$\int_{\mathbb{R}^3\setminus B_{r+t}(0)} d^3\mathbf{x}\,\psi^\dagger(t,\mathbf{x})\psi(t,\mathbf{x}) = -\int_{S_L} d\sigma(x)\, n_\mu(x)\overline{\psi}(x)\gamma^\mu\psi(x). \tag{4.98}$$

Now, we have $n_\mu(x)\overline{\psi}(x)\gamma^\mu\psi(x) \geq 0$ for $x \in S_L$ as the Dirac current is time-like or light-like and future-pointing. Thus, the r.h.s. is ≤ 0 while the l.h.s. is ≥ 0, so both must be equal to zero. From $\int_{\mathbb{R}^3\setminus B_{r+t}(0)} d^3\mathbf{x}\,\psi^\dagger(t,\mathbf{x})\psi(t,\mathbf{x}) = 0$ we conclude, as the integrand is non-negative, that $\psi(t,\mathbf{x}) = 0$ for $\mathbf{x} \in \mathbb{R}^3\setminus B_{r+t}(0)$. This is equivalent to $\operatorname{supp}\psi(t,\cdot) \subset B_{r+t}(0)$. □

Plane wave solutions. Similarly as for the KG equation, we are looking for solutions of the form

$$\psi(x) = u(p)\, e^{-ip_\mu x^\mu}. \tag{4.99}$$

Here, $u : \mathbb{R}^4 \to \mathbb{C}^4$ is a vector-valued function. Plugging in the ansatz (4.99), we obtain the equation

$$(\gamma^\mu p_\mu - m)u(p) = 0. \tag{4.100}$$

This is just a matrix-vector equation with a parameter p. By acting on (4.100) with $(\gamma^\nu p_\nu + m)$, one can see that each component of u satisfies the KG equation. Therefore, we must have

$$p^2 - m^2 = 0 \quad \Leftrightarrow \quad p^0 = \pm\sqrt{\mathbf{p}^2 + m^2}. \tag{4.101}$$

We consider the case $p^0 = +\sqrt{\mathbf{p}^2 + m^2} = \omega(\mathbf{p})$ first and call the respective functions $u(p) =: u_+(\mathbf{p})$. Then (4.100) becomes:

$$(\boldsymbol{\alpha} \cdot \mathbf{p} + \beta m)u_+(\mathbf{p}) = \omega(\mathbf{p})u_+(\mathbf{p}). \tag{4.102}$$

In our representation of the α, β-matrices this is equivalent to the following two equations for $(u_1, u_2) = u_+$:

$$\boldsymbol{\sigma} \cdot \mathbf{p}u_2 + mu_1 = \omega(\mathbf{p})u_1, \tag{4.103}$$

$$\boldsymbol{\sigma} \cdot \mathbf{p}u_1 - mu_2 = \omega(\mathbf{p})u_2. \tag{4.104}$$

As $\omega(\mathbf{p}) > 0 > -m$, this can be easily solved for u_2:

$$u_2(\mathbf{p}) = \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{\omega(\mathbf{p}) + m} u_1(\mathbf{p}). \tag{4.105}$$

Inserting this back into (4.103), we obtain:

$$\left(\frac{(\boldsymbol{\sigma} \cdot \mathbf{p})^2}{\omega(\mathbf{p}) + m} + m \right) u_1 = \omega(\mathbf{p})u_1. \tag{4.106}$$

Now, we have $(\boldsymbol{\sigma} \cdot \mathbf{p})^2 = \mathbf{p}^2$ and

$$\frac{\mathbf{p}^2}{\omega(\mathbf{p}) + m} = \frac{\omega(\mathbf{p})^2 - m^2}{\omega(\mathbf{p}) + m} = \omega(\mathbf{p}) - m. \tag{4.107}$$

Therefore, (4.103) holds identically. We thus have found a class of solutions of the Dirac equation, one for each $\mathbf{p}$ and each u_1. As u_1 has two components, there are two linearly independent solutions $u_+^{(i)}$, $i = 1, 2$ for each $\mathbf{p}$:

$$u_+^{(i)}(\mathbf{p}) = \sqrt{\frac{\omega(\mathbf{p}) + m}{2\omega(\mathbf{p})}} \begin{pmatrix} \chi_i \\ \frac{\boldsymbol{\sigma} \cdot \mathbf{p}}{\omega(\mathbf{p}) + m} \chi_i \end{pmatrix}, \quad i = 1, 2. \tag{4.108}$$

Here, $\chi_1 = (1, 0)$ and $\chi_2 = (0, 1)$, and prefactor of the vector is a normalization constant such that $(u_+^{(i)}(\mathbf{p}))^\dagger u_+^{(i)}(\mathbf{p}) = 1$.

Now we turn to the case $p^0 = -\omega(\mathbf{p})$. As the KG equation, **the Dirac equation also admits negative energies.** We call the respective solutions $u_-(\mathbf{p})$. Proceeding similarly as above, we obtain the following two linearly independent solutions for each $\mathbf{p}$:

$$u_-^{(i)}(\mathbf{p}) = \sqrt{\frac{\omega(\mathbf{p})+m}{2\omega(\mathbf{p})}} \begin{pmatrix} -\frac{\boldsymbol{\sigma}\cdot\mathbf{p}}{\omega(\mathbf{p})+m}\chi_i \\ \chi_i \end{pmatrix}, \quad i = 1, 2, \tag{4.109}$$

where again $\chi_1 = (1, 0)^T$ and $\chi_2 = (0, 1)^T$.

Accordingly, a large class of solutions of the Dirac equation can be obtained by superposing these plane-wave solutions. For $\phi_+, \phi_- \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$

$$\psi(t, \mathbf{x}) = \sum_{j=1,2} \int \frac{d^3\mathbf{p}}{(2\pi)^3} \left(\phi_+(\mathbf{p})\, u_+^{(j)}(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x} - i\omega(\mathbf{p})t} + \phi_-(\mathbf{p}) u_-^{(j)}(\mathbf{p}) e^{i\mathbf{p}\cdot\mathbf{x} + i\omega(\mathbf{p})t} \right) \tag{4.110}$$

yields a solution of the Dirac equation.

Discussion of negative energies, Dirac sea. For the KG equation, negative energy solutions were problematic mainly because then the 0-component of the KG current could become negative. For the Dirac equation, we have

$$j^0 = \psi^\dagger \psi \geq 0 \tag{4.111}$$

independently of whether ψ is a negative energy solution or not. The probability interpretation is therefore not affected by negative energies. Thus, at least the basic logical framework of how we would like to use the Dirac equation is consistent.

However, one might worry that negative energies could cause a different problem. Namely, if the Dirac equation gets coupled to other matter or fields, could one not generate infinite amounts of energy if the Dirac particle lowers its energy infinitely and emits it in form of radiation? Whether or not this really happens, has (to the best of my knowledge) never been analyzed comprehensively. The answer may also depend on the type of interaction between light and matter. Usually, it is described by quantum electrodynamics. We shall not treat this theory here. The general feeling, however, is that the aforementioned infinite lowering of energies could indeed happen, and has to be prevented by some mechanism as one does not observe it in nature.

To prevent the problem, Dirac postulated that for a multi-electron system, there would be infinitely many electrons occupying[3] the negative energy states. This infinity of negative energy electrons has been called **Dirac sea.** If all the negative energy states were occupied, additional electrons with positive energies could not lower their energy below their rest energy mc^2 due to the Pauli principle. The great majority of the Dirac sea could then not interact with positive energy electrons (only those just below $E = -m^2$) and would thus not be seen in experiments. Dirac furthermore showed that if one of the negative energy states is unoccupied, it can be described by the charge conjugated Dirac equation. Dirac first thought this charge conjugated equation would describe the proton. However, it quickly turned out

[3] "Occupying" is meant in the sense of second quantization and the occupation number representation of states in Fock space.

that this could not be the case (due to the mass) and that it instead describes an anti-electron, the positron. Historically, anti-particles were found experimentally shortly after Dirac's discoveries. Besides showing that spin is logically necessary for relativistic wave functions, the prediction of anti-particles is one of the greatest successes of the Dirac equation.

In the prevailing interpretation of quantum electrodynamics, one re-defines the Dirac sea as the vacuum state and treats the absence of a particle in the Dirac sea as its own type of particle, the positron. The transition of a negative energy electron in the Dirac sea to positive energies (leaving back a hole in the Dirac sea) then gets re-interpreted as the creation of an electron-anti-electron pair (both with positive energies). The two views can be translated into each other and are (more or less) mathematically (though not conceptually) equivalent.

4.5 Solution theory

4.5.1 Classical solutions

In this section, we are looking for solutions $\psi \in C^1(\mathbb{R}^4, \mathbb{C}^4)$ of the initial value problem

$$\begin{cases} \psi(0, \mathbf{x}) = \psi_0(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3, \\ (i\gamma^\mu \partial_\mu - m)\psi(t, x) = 0, \quad t \neq 0, \mathbf{x} \in \mathbb{R}^3, \end{cases} \tag{4.112}$$

where $\psi_0 \in C^1(\mathbb{R}^3, \mathbb{C}^4) \cap L^2(\mathbb{R}^3, \mathbb{C}^4)$ is a given function.

First, we prove the uniqueness of the solution.

Theorem 4.5.1 *Let $\psi_1, \psi_2 \in C^1(\mathbb{R}^4, \mathbb{C}^4)$ be a solution of (4.112) such that their restrictions $\psi_{i|_\Sigma}$, $i = 1, 2$ lie in $L^2(\Sigma, \mathbb{C}^4)$ for every space-like hyperplane $\Sigma \subset \mathbb{M}$. Then we have $\psi_1 = \psi_2$.*

Proof: You have already shown this on **Sheet 6, Exercise 3** using the technique of "energy" integrals applied to the total probability integral $P(\Sigma) = \int_\Sigma d\sigma(x)\, n_\mu(x) \overline{\psi}(x) \gamma^\mu \psi(x)$.

Next, we show that *provided there exists a solution* of (4.112), it can be found via reduction to a KG equation with special initial data.

Theorem 4.5.2 *Let $\psi_0 \in C^3(\mathbb{R}^3, \mathbb{C}^4)$ and assume the IVP (4.112) has a solution $\psi \in C^2(\mathbb{R}^4, \mathbb{C}^4)$ such that for every space-like hyperplane $\Sigma \subset \mathbb{M}$, the restriction $\psi_{|_\Sigma}$ lies in $L^2(\Sigma, \mathbb{C}^4)$. Then the solution is unique and its spin components ψ_j, $j = 1, 2, 3, 4$ are given by*

$$\begin{aligned} \psi_j(\tau, \mathbf{y}) = {} & \frac{\tau}{4\pi} \int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, g_j(\mathbf{x} + \mathbf{y}) - \frac{m}{4\pi} \int_{B_\tau(0)} d^3\mathbf{x}\, \frac{J_1(m\sqrt{\tau^2 - |\mathbf{x}|^2})}{\sqrt{\tau^2 - |\mathbf{x}|^2}} g_j(\mathbf{x} + \mathbf{y}) \\ & + \frac{\partial}{\partial \tau} \left(\frac{\tau}{4\pi} \int_{\partial B_\tau(0)} d\Omega_{\mathbf{x}}\, f_j(\mathbf{x} + \mathbf{y}) - \frac{m}{4\pi} \int_{B_\tau(0)} d^3\mathbf{x}\, \frac{J_1(m\sqrt{\tau^2 - |\mathbf{x}|^2})}{\sqrt{\tau^2 - |\mathbf{x}|^2}} f_j(\mathbf{x} + \mathbf{y}) \right), \end{aligned} \tag{4.113}$$

where for $j = 1, 2, 3, 4$

$$f_j(\mathbf{x}) = (\psi_0)_j(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3 \tag{4.114}$$

and

$$g_j(\mathbf{x}) = -i(\alpha^k \partial_k \psi_0)_j(\mathbf{x}) + m(\beta\psi_0)_j(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^3. \tag{4.115}$$

Proof: We already know that under the given conditions, the solution ψ is unique. Furthermore, as $\psi \in C^2(\mathbb{R}^4, \mathbb{C}^4)$, each component ψ_j solves the KG equation. The initial data are given by (4.114) and by (4.115). The latter can be seen by differentiating ψ w.r.t. t and using the fact that ψ is a solution of the Dirac equation. By theorems 3.3.1 and 3.3.2, we obtain that the unique solution of the initial value problem of the KG equation for the j-th component is given by (4.113), $j = 1, 2, 3, 4$. Here, the regularity property $\psi_0 \in C^3(\mathbb{R}^3, \mathbb{C}^4)$ is required. Now, as the IVP of the Dirac equation has by assumption one solution (and by uniqueness exactly one) which also satisfies the IVP of the KG equation, this solution coincides with (4.113). □

Remark. With some effort, one can also demonstrate directly that the formula (4.113) yields a solution (i.e., without relying on the a-priori assumption that a C^2-solution of the Dirac equation exists).

4.5.2 Hilbert space valued solutions

In this section we study a more abstract notion of solution of the Dirac equation which is common in mathematical physics and functional analysis.

Hamiltonian formulation of the Dirac equation. By multiplying the Dirac equation with γ^0, one can rewrite it as follows:

$$i\partial_t \psi(t, \mathbf{x}) = H^{\text{Dirac}} \psi(t, \mathbf{x}) \tag{4.116}$$

with the Dirac Hamiltonian

$$H^{\text{Dirac}} = -i\alpha^j \partial_j + m\beta \quad \text{(sum over } j = 1, 2, 3). \tag{4.117}$$

One now interprets (4.116) as an equation on Hilbert space,

$$\mathscr{H} = L^2(\mathbb{R}^3, \mathbb{C}^4) \tag{4.118}$$

with scalar product

$$\langle \psi, \phi \rangle = \int d^3\mathbf{x}\, \psi^\dagger(\mathbf{x}) \varphi(\mathbf{x}). \tag{4.119}$$

Note that the functions $\psi \in \mathscr{H}$ are time-independent. (The Hilbert space formulation is therefore not manifestly Lorentz invariant.) One thus interprets the wave function $\psi(t, \mathbf{x})$ in the Dirac equation as a map

$$\psi : \mathbb{R} \to \mathscr{H}, \quad t \mapsto \psi(t). \tag{4.120}$$

The Dirac equation is then to be understood as an ordinary differential equation for the Hilbert space valued map $\psi(t)$ as follows:

$$i\frac{d\psi(t)}{dt} = H^{\text{Dirac}} \psi(t). \tag{4.121}$$

H^{Dirac} is, as usual for differential operators, an unbounded operator on $\mathscr{H}$. It can thus not be defined on the whole of $\mathscr{H}$ but only on a certain domain, $\mathscr{D}(H^{\text{Dirac}}) \subset \mathscr{H}$. It turns out that for the Dirac operator, a suitable domain is given by

$$\mathscr{D}(H^{\text{Dirac}}) = H^1(\mathbb{R}^3)^4, \tag{4.122}$$

the *first Sobolev space* of functions from $\mathbb{R}^3$ to $\mathbb{C}^4$. (This means, one can take the first weak derivatives of ψ in the spatial directions.)

The goal now is to show that H^{Dirac} is self-adjoint on $\mathscr{D}(H^{\text{Dirac}})$. Then, by *Stone's theorem*,

$$U(t) = \exp(-iH^{\text{Dirac}}t) \tag{4.123}$$

defines a strongly continuous unitary one-parameter group on $\mathscr{H}$. Furthermore, we have:

$$i\frac{dU(t)}{dt}\bigg|_{t=0} = H^{\text{Dirac}}. \tag{4.124}$$

Thus, (4.121) with initial condition $\psi(0) = \psi_0 \in \mathscr{H}$ has the unique solution

$$\psi(t) = U(t)\psi_0. \tag{4.125}$$

Indeed, we have the following theorem (Thaller p. 11):

Theorem 4.5.3 *H^{Dirac} is self-adjoint on the first Sobolev space*

$$\mathscr{D}(H^{\text{Dirac}}) = H^1(\mathbb{R}^3)^4. \tag{4.126}$$

Its spectrum is purely continuous[4] *and given by*

$$\sigma(H^{\text{Dirac}}) = (-\infty, -m] \cup [m, \infty). \tag{4.127}$$

Proof: We first prove the statement about self-adjointness and spectrum. The idea is to reduce the problem to a multiplication operator with a self-adjoint matrix via Fourier transformation (similarly as for the plane-wave solutions of the Dirac equation). Let $\mathcal{F}$ denote the Fourier transformation. $\mathcal{F}$ is first defined on integrable (L^1) functions but can be uniquely extended to a unitary operator on $\mathscr{H} = L^2(\mathbb{R}^3)^4$. For the Dirac operator, we have:

$$(\mathcal{F}H^{\text{Dirac}}\mathcal{F})(\mathbf{p}) = h(\mathbf{p}) := \begin{pmatrix} m\,\mathbb{1}_2 & \boldsymbol{\sigma}\cdot\mathbf{p} \\ \boldsymbol{\sigma}\cdot\mathbf{p} & -m\,\mathbb{1}_2 \end{pmatrix}. \tag{4.128}$$

For each $\mathbf{p}$, this is a Hermitian 4×4 matrix with eigenvalues

$$\lambda_1(|\mathbf{p}|) = \lambda_2(|\mathbf{p}|) = -\lambda_3(|\mathbf{p}|) = -\lambda_4(|\mathbf{p}|) = \sqrt{\mathbf{p}^2 + m^2} = \omega(\mathbf{p}). \tag{4.129}$$

As $h(\mathbf{p})$ is Hermitian, there is a unitary transformation $u(\mathbf{p})$ which diagonalizes $h(\mathbf{p})$. Explicitly:

$$u(\mathbf{p}) = \frac{(m+\omega(\mathbf{p}))\mathbb{1}_4 + \beta\,\boldsymbol{\alpha}\cdot\mathbf{p}}{\sqrt{2\omega(\mathbf{p})(m+\omega(\mathbf{p}))}}. \tag{4.130}$$

[4]The continuous spectrum of an operator A on $\mathscr{H}$ is defined as those $\lambda \in \mathbb{C}$ which make the range of $A - \lambda\,\mathbb{1}$ a proper dense subset of $\mathscr{H}$.

Then:

$$u(\mathbf{p})h(\mathbf{p})u(\mathbf{p})^{-1} = \beta\,\omega(\mathbf{p}). \tag{4.131}$$

Overall, we see that unitary the operator

$$\mathcal{W} = u\,\mathcal{F} \tag{4.132}$$

converts H^{Dirac} into a multiplication operator with a diagonal matrix

$$(\mathcal{W}H^{\text{Dirac}}\mathcal{W}^{-1})(\mathbf{p}) = \beta\,\omega(\mathbf{p}) \tag{4.133}$$

on the Hilbert space $L^2(\mathbb{R}^3, d^3\mathbf{p})$.
Because of this unitary equivalence to this self-adjoint multiplication operator, H^{Dirac} itself is self-adjoint on

$$\mathscr{D}(H^{\text{Dirac}}) = \mathcal{W}^{-1}\mathscr{D}(\beta\,\omega(\cdot)) = \mathcal{F}^{-1}u^{-1}\mathscr{D}(\omega(\cdot)) = \mathcal{F}^{-1}\mathscr{D}(\omega(\cdot)). \tag{4.134}$$

The last step follows as u^{-1} is a multiplication operator with a unitary matrix which does not change the domain of a multiplication operator.
Now the first Sobolev space $H^1(\mathbb{R}^3)^4$ is by definition given by the inverse Fourier transformation of the set

$$\{f \in L^2(\mathbb{R}^3, d^3\mathbf{p})^4 : (1+|\mathbf{p}|^2)^{1/2} f \in L^2(\mathbb{R}^3, d^3\mathbf{p})^4\}. \tag{4.135}$$

As $\omega(\mathbf{p}) = \sqrt{m^2+|\mathbf{p}|^2}$, this set equals $\mathscr{D}(\omega(\cdot))$ (for $m \neq 0$).

Similarly, the spectrum of H^{Dirac} is given by the spectrum of the multiplication operator $\beta\omega(\cdot)$ which is given by $(-\infty, -m] \cup [m, \infty)$. □

Representation of the solution by an integral formula.

Theorem 4.5.4 (Thaller p. 15) *Let $\psi_0 \in \mathcal{S}(\mathbb{R}^3)^4$ (the set of rapidly decreasing* Schwarz functions *with four components). Then for $t \neq 0$, the unique solution ψ of the Dirac equation with initial data $\psi(0,\cdot) = \psi_0(\cdot)$ is given by:*

$$\psi(t,\mathbf{x}) = -i\int_{\mathbb{R}^3} d^3\mathbf{y}\, S(t,\mathbf{x}-\mathbf{y})\gamma^0\psi_0(\mathbf{y}), \tag{4.136}$$

where $S(t,\mathbf{x})$ is the distribution given by

$$S(t,\mathbf{x}) = (i\gamma^\mu\partial_\mu + m)\Delta(x) \tag{4.137}$$

and

$$\Delta(x) = \frac{\operatorname{sgn}(x^0)}{2\pi}\left[\delta(x_\mu x^\mu) - \frac{m}{2}\theta(x_\mu x^\mu)\frac{J_1(m\sqrt{x_\mu x^\mu})}{\sqrt{x_\mu x^\mu}}\right]. \tag{4.138}$$

For the proof, see Thaller pp. 16-18 (note the different sign conventions).

Remarks.

1. The representation formula for the solution (4.136) can be shown to be identical to our previous result (4.113), at least for $t > 0$.

2. The formula (4.136) is the analog of the solution formula (3.44) for the KG equation via its retarded Green's function.

3. $S(t, \mathbf{x})$ is the called the *propagator* of the Dirac equation. For $t > 0$, $S(t, \mathbf{x})$ coincides with the retarded Green's function $S^{\text{ret}}(t, \mathbf{x})$ of the Dirac equation, and for $t < 0$ with minus the advanced Green's function $-S^{\text{adv}}(t, \mathbf{x})$.

4. One obtains Green's functions of the Dirac equation from those of the KG equation by applying the operator $-(i\gamma^\mu \partial_\mu + m)$:

$$S^{(i)}(x) = -(i\gamma^\mu \partial_\mu + m) G^{(i)}(x) \tag{4.139}$$

   where $G^{(i)}(x)$ is a Green's function of the KG equation.

5. $\Delta(x) = G^{\text{ret}}(x) - G^{\text{adv}}(x)$, where G^{ret}, G^{adv} are retarded and advanced Green's functions of the KG equation, respectively. So for $x^0 > 0$, $\Delta(x) = G^{\text{ret}}(x)$ which agrees exactly with the distribution K we used for the solution of initial value problem for the KG equation and $t > 0$.

Generalization of the representation formula to arbitrary space-like hyperplanes. For every space-like hyperplane $\Sigma \subset \mathbb{M}$ with future-pointing unit normal vector field n and every $\psi_\Sigma \in \mathcal{S}(\Sigma)^4$, the unique solution of the initial value problem

$$\psi(x) = \psi_\Sigma(x), \quad x \in \Sigma \tag{4.140}$$

of the Dirac equation is given by:

$$\psi(x) = -i \int_\Sigma d\sigma(y)\, S(x-y) \gamma^\mu n_\mu(y)\, \psi_\Sigma(y). \tag{4.141}$$

By using this formula (i) for $x \in \Sigma$ or (ii) repeatedly for two different hyperplanes Σ, Σ', we obtain the following distributional identities (**Sheet 10, Exercise 3**):

(i) $S(0, \mathbf{x}) = i\gamma^0 \delta^{(3)}(\mathbf{x})$,

(ii) $-i \int_\Sigma d\sigma(y)\, S(x-y) \gamma^\mu n_\mu(y) S(y-z) = S(x-z)$ for every space-like hyperplane Σ.

Remark: The formula (4.141) also holds for more general curved space-like hypersurfaces Σ.

Natural Hilbert spaces for the Dirac equation. If we want to have a space-time picture for the Dirac equation, the Hilbert space $\mathscr{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$ is not particularly natural. The fact that probability conservation holds on arbitrary space-like hyperplanes (in fact, on arbitrary space-like Cauchy surfaces) $\Sigma \subset \mathbb{M}$, suggests to define the following Hilbert spaces:

$$\mathscr{H}_\Sigma = L^2(\Sigma, \mathbb{C}^4, d\sigma(x)) \tag{4.142}$$

with scalar product ($\rightarrow$ **Sheet 10, Exercise 2**):

$$\langle \psi, \varphi \rangle_\Sigma = \int_\Sigma d\sigma(x)\, n_\mu(x) \overline{\psi}(x) \gamma^\mu \varphi(x). \tag{4.143}$$

This defines a norm in the usual way,

$$\|\psi\|_\Sigma = \sqrt{\langle \psi, \psi \rangle_\Sigma}. \tag{4.144}$$

Then, evaluating the solution formula (4.141) for x on a space-like hyperplane Σ' defines an injective map

$$U_\Sigma^{\Sigma'} : \mathcal{S}(\Sigma)^4 \to \mathscr{H}_{\Sigma'}. \tag{4.145}$$

Total probability conservation means that

$$\|\psi_{|\Sigma}\|_\Sigma = \|\psi_{|\Sigma'}\|_{\Sigma'} = \|U_\Sigma^{\Sigma'} \psi_{|\Sigma}\|_{\Sigma'}. \tag{4.146}$$

Together with the uniqueness of the solution this suggests that U can be extended to a unitary map between the full Hilbert spaces $\mathscr{H}_\Sigma$ and $\mathscr{H}_{\Sigma'}$, i.e.

$$U_\Sigma^{\Sigma'} : \mathscr{H}_\Sigma \to \mathscr{H}_{\Sigma'}. \tag{4.147}$$

The previous unitary operator $U(t) = \exp(-iH^{\text{Dirac}}t)$ can be thought of as the special case of $U_\Sigma^{\Sigma'}$ for $\Sigma = \Sigma_{t=0}$ and $\Sigma' = \Sigma_t$. One should note that the Hilbert spaces $\mathscr{H}_{\Sigma_t}$ can, for every $t \in \mathbb{R}$, be canonically identified with $\mathscr{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$, namely through

$$\mathscr{H}_{\Sigma_t} \ni \psi_{|\Sigma_t} \equiv \psi(t, \cdot) \in \mathscr{H}. \tag{4.148}$$

5. The multi-time formalism

In this chapter, we are concerned with the description of many relativistic quantum particles.

5.1 Motivation

The usual way to a many-body quantum theory in the Schrödinger picture. The usual way from a single-particle to a many-particle quantum theory is to take tensor products of the single-particle Hilbert spaces and to take the sum of the Hamiltonians as the overall free (non-interacting) Hamiltonian.

We consider the case of N particles, each described by a Dirac equation (with possibly different masses). The (time-independent) Hilbert space then is $\mathscr{H} = L^2(\mathbb{R}^3, \mathbb{C}^4)$, and its N-fold tensor product yields:

$$\mathscr{H}^{\otimes N} \cong L^2(\mathbb{R}^{3N}, \mathbb{C}^{4^N}). \tag{5.1}$$

The idea is that the wave function, φ, then satisfies the Schrödinger equation

$$i\frac{d\varphi(t)}{dt} = \sum_{k=1}^{N} H_k^{\text{Dirac}}\, \varphi(t) + V\varphi(t) \tag{5.2}$$

where

$$H_k^{\text{Dirac}} = \sum_{j=1}^{3}(-i\gamma_k^0\gamma_k^j\partial_{k,j}) + \gamma_k^0 m_k \tag{5.3}$$

with $\partial_{k,\mu} = \frac{\partial}{\partial x_k^\mu}$ and

$$\gamma_k^\mu = \mathbb{1} \times \cdots \otimes \mathbb{1} \underbrace{\otimes \gamma^\mu \otimes}_{k\text{-th place}} \mathbb{1} \otimes \cdots \otimes \mathbb{1}. \tag{5.4}$$

Moreover, $\hat{V}$ is a multiplication operator with a function $V(t, \mathbf{x}_1, ..., \mathbf{x}_N)$ with values in the symmetric matrices.

Overall, that means φ has to be viewed as a map

$$\varphi : \mathbb{R} \times \mathbb{R}^{3N} \to (\mathbb{C}^4)^{\otimes N} \cong \mathbb{C}^{4^N}, \quad (t, \mathbf{x}_1, ..., \mathbf{x}_N) \mapsto \varphi(t, \mathbf{x}_1, ..., \mathbf{x}_N). \tag{5.5}$$

We call this map the *single-time wave function*.

When formulated as a PDE (instead of as an ODE on Hilbert space), the Schrödinger equation becomes:

$$i\partial_t\varphi = \sum_{k=1}^{N} \left(-i\gamma_k^0\gamma_k^j\partial_{k,j} + \gamma_k^0 m_k\right)\varphi + V(t, \mathbf{x}_1, ..., \mathbf{x}_N)\varphi. \tag{5.6}$$

Limitation of the usual approach. Our goal is to obtain a relativistic theory. However, the above approach suffers from the following problems (for $N \geq 2$):

1. It is not clear how to Lorentz-transform the single-time wave function. This is because the argument $(t, \mathbf{x}_1, ..., \mathbf{x}_N)$ contains N spatial variables but only one time. For such variables, there is no pre-defined transformation behavior under Lorentz boosts. (For rotation, on the other hand, we could rotate each $\mathbf{x}_i$ in the same way.)

2. Relatedly, the single-time Schrödinger equation (5.6) is not manifestly Lorentz invariant.

3. The Born rule corresponding to the outlined theory is:

   > $(\varphi^\dagger\varphi)(t, \mathbf{x}_1, ..., \mathbf{x}_N)\, d^3\mathbf{x}_1 \cdots d^3\mathbf{x}_N$ is the probability to find N particles, each particle i at a location in the infinitesimal volume $d^3\mathbf{x}_i$ around $\mathbf{x}_i \in \mathbb{R}^3$ at time t.

   As this statement refers to a particular time coordinate t, it only holds for one particular Lorentz frame. We would like to have a frame-independent statement instead.

Derivation of multi-time wave functions from Lorentz transformations of configurations. We now give an argument in favor of a relativistic type of wave function which overcomes the above-mentioned problems.

From the Born rule, we can see that the argument of φ, $(t, \mathbf{x}_1, ..., \mathbf{x}_N)$ refers to a spatial configuration $(\mathbf{x}_1, ..., \mathbf{x}_N) \in \mathbb{R}^3$ at a certain time t. The same space-time configuration is expressed by the following collection of 4-vectors:

$$((t, \mathbf{x}_1), ..., (t, \mathbf{x}_N)). \tag{5.7}$$

Given this collection of 4-vectors, it is now clear how a Lorentz transformation Λ acts, namely by applying Λ to each 4-vector:

$$((t, \mathbf{x}_1), ..., (t, \mathbf{x}_N)) \overset{\Lambda}{\to} (\Lambda(t, \mathbf{x}_1), ..., \Lambda(t, \mathbf{x}_N)) = ((t'_1, \mathbf{x}'_1), ..., (t'_N, \mathbf{x}'_N)). \tag{5.8}$$

The important point is that in general, $t'_j \neq t'_k$ for $j \neq k$. So we end up with N *different time variables* after the Lorentz transformation.

We now want to apply this insight to the argument of the wave function. To this end, we must first identify $\varphi(t, \mathbf{x}_1, ..., \mathbf{x}_N)$ as the equal-time case of a more general object $\psi(t_1, \mathbf{x}_N, ..., t_N, \mathbf{x}_N)$ which may exist for $t_j \neq t_k$, i.e.:

$$\varphi(t, \mathbf{x}_1, ..., \mathbf{x}_N) = \psi(t, \mathbf{x}_1, ..., t, \mathbf{x}_N). \tag{5.9}$$

Recalling the transformation behavior of the wave function of the Dirac equation (4.41), we expect the following transformation behavior:

$$\psi'(x'_1, ..., x'_N) = S[\Lambda]^{\otimes N} \psi(x_1, ..., x_N). \tag{5.10}$$

This implies:

$$\psi'(t,\mathbf{x}_1,...,t,\mathbf{x}_N) = S[\Lambda]^{\otimes N}\psi(\Lambda^{-1}(t,\mathbf{x}_1),....,\Lambda^{-1}(t,\mathbf{x}_N)) = S[\Lambda]^{\otimes N}\psi(t'_1,\mathbf{x}'_1,...,t'_N,\mathbf{x}'_N), \tag{5.11}$$

where in general $t'_j \neq t'_k$ for $j \neq k$ (here $x'_i = \Lambda^{-1}x_i$). So we find that ψ *is indeed needed on space-time configurations with different times.*

Definition: Let $N \in \mathbb{N}$, $N \geq 2$ be the number of particles and $K \in \mathbb{N}$ the number of spin components per particle. Moreover, let Ω be a Poincaré invariant[1] subset of $\mathbb{R}^{4N}$. Then a *multi-time wave function* is a map

$$\psi : \Omega \subset \mathbb{R}^{4N} \to \mathbb{C}^{K^N}, \quad (x_1,...,x_N) \mapsto \psi(x_1,...,x_N). \tag{5.12}$$

Remark. Natural choices for Ω are $\Omega = \mathbb{R}^{4N}$ and $\Omega = \mathscr{S}$, the set of *space-like configurations:*

$$\mathscr{S} = \{(x_1,...,x_N) \in \mathbb{R}^{4N} : \forall j \neq k : (x_j - x_k)_\mu (x_j - x_k)^\mu < 0\}. \tag{5.13}$$

You will show on **Sheet 11, Exercise 2** that for $N = 2$, $\mathscr{S}$ is the smallest Poincaré invariant set which contains the equal-time collision-free configurations $C = \{(x_1,...,x_N) \in \mathbb{R}^{4N} : x_i = x_j \,\forall i,j \text{ and } \mathbf{x}_j \neq \mathbf{x}_k \,\forall j \neq k\}$.

Historical Remark. The idea of multi-time wave functions dates back to Dirac's paper

> P. A. M. Dirac, *Relativistic Quantum Mechanics*, Proc. R. Soc. Lond. A, 136:453–464, 1932.

A recent overview of the theory of multi-time wave functions can be found in:

> M. Lienert, S. Petrat, and R. Tumulka. *Multi-time wave functions.* J. Phys. Conf. Ser., 880(1):012006, 2017. `https://doi.org/10.1088/1742-6596/880/1/012006`

5.2 Evolution equations

Multi-time Schrödinger equations. A multi-time wave function has N time coordinates. Therefore, it was Dirac's idea that one needs one evolution equation for each time coordinate. This leads to a system of N equations which ψ needs to satisfy simultaneously:

$$\begin{aligned} i\partial_{t_1}\psi &= H_1\psi, \\ &\vdots \\ i\partial_{t_N}\psi &= H_N\psi. \end{aligned} \tag{5.14}$$

[1] A Poincaré transformation (a,Λ) acts on $(x_1,...,x_N) \in \mathbb{R}^{4N}$ as $(\Lambda x_1 + a,...,\Lambda x_N + a)$.

Here, $t_i = x_i^0$. It is understood that one should be able to rewrite (5.14) in a manifestly Lorentz invariant form, such as in the example of free multi-time Dirac equations:

$$(i\gamma_k^\mu \partial_{k,\mu} - m_k)\psi(x_1, ..., x_N) = 0, \quad k = 1, ..., N. \tag{5.15}$$

You will analyze these equations in more detail on **Sheet 11, Exercise 1.**

The operators H_k in (5.14) are supposed to be differential operators on an appropriate function space. There are different ways to interpret the system (5.14) mathematically. Perhaps the most appropriate and straightforward way is as a system of N partial differential equations. Alternatively, one can also view it as a system of N equations for a Hilbert space valued function of N time variables,

$$\psi : \mathbb{R}^N \to \mathscr{H}, \quad (t_1, ..., t_N) \mapsto \psi(t_1, ..., t_N) \in \mathscr{H}. \tag{5.16}$$

Note that in this view, the choice $\mathscr{H} = L^2(\mathbb{R}^{3N}, \mathbb{C}^{4^N})$ distinguishes a particular Lorentz frame which is, from a relativistic standpoint, not very natural. However, one can still use it as a mathematical convenience (bearing in mind that the involved frame is somewhat arbitrary).

We re-obtain the familiar single-time Schrödinger equation from the multi-time equations (5.14) by considering $i\partial_t \varphi(t) = i\partial_t \psi(t, \cdots, t)$ and using the chain rule:

$$i\partial_t \psi(t, \cdots, t) = \sum_{k=1}^{N} H_k \psi(t, ..., t). \tag{5.17}$$

That means, the operators H_k sum up to the Hamiltonian of the system. They are therefore called *partial Hamiltonians*.

Initial data. The role of the multi-time equations (5.14) is to determine ψ uniquely given initial data on a set of the form Σ^N where $\Sigma \subset \mathbb{M}$ is a Cauchy surface. Perhaps most conveniently, one can choose $\Sigma = \Sigma_{t=0}$ in a particular Lorentz frame. Then initial data are given by

$$\psi(0, \mathbf{x}_1, ..., 0, \mathbf{x}_N) = \psi_0(\mathbf{x}_1, ..., \mathbf{x}_N), \quad \mathbf{x}_i \in \mathbb{R}^3, i = 1, ..., N \tag{5.18}$$

for some given function $\psi_0 : \mathbb{R}^{3N} \to \mathbb{C}^{K^N}$.

Now the crucial question is: when is it possible to uniquely solve (5.14) for all initial data (5.18)? This is an important question, as (5.14) is a system of N simultaneous PDEs which might not always have a solution. We shall now work out conditions when this is possible. We start with the Hilbert space view, and the case that the partial Hamiltonians H_k can be viewed as time-independent operators on Hilbert space.

Consistency conditions.

Definition: Let $\mathscr{H}$ be a Hilbert space. A *strongly continuous unitary N-parameter group* is a map U from $\mathbb{R}^N$ into the set of unitary operators on $\mathscr{H}$ such that $U(0) = \mathbb{1}$ and for $\mathbf{t}, \mathbf{s} \in \mathbb{R}^N$: $U(\mathbf{t})U(\mathbf{s}) = U(\mathbf{t} + \mathbf{s})$. Furthermore, *strongly continuous* means that each one-parameter subgroup $U_j(t_j) = U(0, ..., 0, t_j, 0, ..., 0)$ is strongly continuous. According to the theorem of Stone this means that $i\frac{d}{dt_j} U_j(t_j)|_{t_j=0}$ exists and is given by a self-adjoint operator.

Definition: We say that the multi-time equations (5.14) have a *Hilbert-space valued solution* for all initial data $\psi_0 \in \mathscr{H}$ if and only if there exists a strongly continuous unitary N-parameter group $U(t_1, ..., t_N)$ with

$$i\frac{\partial}{\partial t_j}U(0, ..., 0, t_j, 0, ..., 0) = H_j\, U(0, ..., 0, t_j, 0, ..., 0). \tag{5.19}$$

(Then the solution is given by $\psi(t_1, ..., t_N) = U(t_1, ..., t_N)\psi_0$.)

Theorem 5.2.1 *Let $\mathscr{H}$ be a Hilbert space and $H_1, ..., H_N$ be time-independent self-adjoint operators on $\mathscr{H}$. Then there exists a Hilbert-space valued solution of the initial value problem*

$$\begin{cases} \psi(0, ..., 0) = \psi_0 \in \mathscr{H}, \\ i\partial_{t_k}\psi(t_1, ..., t_N) = H_k\psi(t_1, ..., t_N), \quad k = 1, ..., N\psi, \quad t_1, ..., t_N \in \mathbb{R} \end{cases} \tag{5.20}$$

for all initial data $\psi_0 \in \mathscr{H}$ if and only if

$$[H_j, H_k] = 0 \ \forall j \neq k \tag{5.21}$$

(in the spectral sense)[2].

Proof: "⇒" For $j, k = 1, ..., N, j \neq k$, let H_j be self-adjoint and let $[H_j, H_k] = 0$ in the spectral sense (all spectral projections from the spectral theorem of these self-adjoint operators commute). The self-adjointness of each H_j allows us to define the strongly continuous unitary one-parameter groups

$$U_j(t_j) = e^{-iH_j t_j}. \tag{5.22}$$

Because of (5.21), these groups commute with each other for $j \neq k$. That means that

$$U(t_1, ..., t_N) = e^{-iH_1 t_1} \cdots e^{-iH_N t_N} \tag{5.23}$$

defines a strongly continuous unitary N-parameter group. (Note that the different exponentials have to commute to ensure this.) Moreover,

$$i\frac{\partial}{\partial t_k}U(t_1, ..., t_N) = H_k U(t_1, ..., t_N). \tag{5.24}$$

Therefore,

$$\psi(t_1, ..., t_N) = U(t_1, ..., t_N)\psi_0 \tag{5.25}$$

is a solution of the IVP (5.20).

"⇐" Let (5.20) have an $\mathscr{H}$-valued solution for all initial data. By the definition of the Hilbert space valued solution, there then exists a strongly continuous unitary N-parameter group $U(t_1, ..., t_N)$ whose one-parameter subgroups $U_j(t_j)$ are given by

[2]This means that all spectral projections of the operators have to commute. See the spectral theorem.

$e^{-iH_j t_j}$ according to Stone's theorem. Then, as $U(\mathbf{t}+\mathbf{s}) = U(\mathbf{t})U(\mathbf{s})$ for all $\mathbf{t}, \mathbf{s} \in \mathbb{R}^N$, we have, for all $j \neq k$:

$$\begin{aligned} U(..., t_j, ..., t_k, ...) &= U_j(t_j)U(..., t_j = 0, ..., t_k, ...) = U_j(t_j)U_k(t_k)U(..., t_j = 0, ..., t_k = 0, ...) \\ &= e^{-iH_j t_j} e^{-iH_k t_k} U(..., t_j = 0, ..., t_k = 0, ...) \end{aligned} \tag{5.26}$$

On the other hand, we obtain analogously:

$$U(..., t_j, ..., t_k, ...) = e^{-iH_k t_k} e^{-iH_j t_j} U(..., t_j = 0, ..., t_k = 0, ...). \tag{5.27}$$

Setting all other $t_l = 0$, this implies $e^{-iH_j t_j} e^{-iH_k t_k} = e^{-iH_k t_k} e^{-iH_j t_j}$ which is equivalent to $[H_j, H_k] = 0$ in the spectral sense. □

Remark. $[H_j, H_k]$ $\forall j \neq k$ is called the *consistency condition* for the multi-time equations (5.14). In the case that the partial Hamiltonians are time-dependent maps $H_j = H(t_1, ..., t_N)$ from $\mathbb{R}^N$ into the self-adjoint operators, the condition gets replaced by[3]

$$[H_j, H_k] - i\frac{\partial H_k}{\partial t_j} + i\frac{\partial H_j}{\partial t_k} = 0 \ \forall j \neq k. \tag{5.28}$$

No-go theorem for potentials. The consistency conditions (5.28) are fairly restrictive. We shall now see that they rule out interaction potentials (even Poincaré invariant ones).

Theorem 5.2.2 *For $k = 1, ..., N$ let*

$$H_k(t_1, ..., t_N) = H_k^{\text{Dirac}} + V_k(x_1, ..., x_N) \tag{5.29}$$

where for each k, $V_k : \mathbb{R}^{4N} \to \mathbb{R}$ is a smooth function. Then:

(i) The consistency conditions (5.28) *are satisfied only if V_k does not depend on $\mathbf{x}_j$ for $j \neq k$, $k, j = 1, ..., N$.*

(ii) If in addition all V_k are Poincaré invariant, then (5.28) *is only satisfied if $V_k = const$ for all $k = 1, ..., N$.*

Proof: (i) We write out the consistency conditions (5.28) in detail in our case. Using that $[V_j, V_k] = 0$ and $[H_j^{\text{Dirac}}, H_k^{\text{Dirac}}] = 0$, we find:

$$\begin{aligned} 0 &= [H_j, H_k] - i\frac{\partial V_k}{\partial t_j} + i\frac{\partial V_j}{\partial t_k} \\ &= [H_j^{\text{Dirac}}, V_k] - [H_k^{\text{Dirac}}, V_j] + i\left(\frac{\partial V_j}{\partial t_k} - \frac{\partial V_k}{\partial t_j}\right) \\ &= -i\sum_{l=1}^{3}\left(\gamma_j^0\gamma_j^l\frac{\partial V_k}{\partial x_j^l} - \gamma_k^0\gamma_k^l\frac{\partial V_j}{\partial x_k^l}\right) + i\left(\frac{\partial V_j}{\partial t_k} - \frac{\partial V_k}{\partial t_j}\right). \end{aligned} \tag{5.30}$$

[3]See S. Petrat and R. Tumulka. J. Math. Phys., 55(032302), 2014.

Now, the matrices $\mathbb{1}, \gamma_j^0\gamma_j^l, \gamma_k^0\gamma_k^l$, $j \neq k$, $l = 1,2,3$ are all linearly independent. Thus their coefficients have to vanish separately and we obtain:

$$\frac{\partial V_j}{\partial t_k} = \frac{\partial V_k}{\partial t_j} \tag{5.31}$$

and

$$\frac{\partial V_k}{\partial x_j^l} = 0, \tag{5.32}$$

$j \neq k = 1, ..., N,\ l = 1,2,3$. (5.32) already shows claim (i).

(ii) Lorentz invariance now implies that V_k must not depend on x_j^0, either, $j \neq k$, $j,k = 1, ..., N$. That means, $V_k(x_1, ..., x_N) = \widetilde{V}_k(x_k)$ for some smooth function $\widetilde{V}_k : \mathbb{R}^4 \to \mathbb{C}$, $k = 1, ..., N$. Then it follows from translation invariance that $V_k = \text{const}$, $k = 1, ..., N$. □

Remarks.

1. The first rigorous result in the spirit of the above theorem was obtained by Petrat and Tumulka[4]. They do not assume Poincaré invariance of the potentials and prove that even for potentials which are not Poincaré invariant the multi-time equations must be gauge equivalent to equations with purely external potentials (no interaction).

2. The above theorem only treats the case of scalar potentials, such as Coulomb potentials $V_j = \frac{1}{2}\sum_{k\neq j} \frac{1}{|\mathbf{x}_j - \mathbf{x}_k|}$ (or a Poincaré invariant version of this). There are also more elaborate versions of the theorem for matrix valued potentials. Perhaps the most complete result is a theorem by Nickel and Deckert.[5] They admit arbitrary matrix-valued potentials $V_j : \mathbb{R}^{4N} \to (\mathbb{C}^4)^{\otimes N}$ and prove that there are no Poincaré invariant ones besides $V_j = 0\,\forall j$ which satisfy the consistency conditions.

3. A similar result also holds for $-\Delta_k$, the k-th Laplacian, instead of H_k^{Dirac}. ($\to$ **Sheet 12, Exercise 1**). This shows that it is really the form of the multi-time system (5.14) which excludes interaction potentials. Poincaré invariance does not play an important role in this.

Conclusion. Potentials are not a viable mechanism for interaction in multi-time equations, and an alternative mechanism is necessary. One such possibility will be presented in Sec. 5.4.

5.3 Probability conservation and generalized Born rule

In this section, we discuss the question how to generalize the Born rule to arbitrary space-like surfaces using a multi-time wave function. Physically, this means we now

[4] See S. Petrat and R. Tumulka. J. Math. Phys., 55(032302), 2014.
[5] L. Nickel and D.-A. Deckert. J. Math. Phys. 57 072301 (2016).

describe the detection probabilities of particles at different times (but such that the detection events remain space-like to each other). The discussion proceeds at the case of a fixed number N of particles.

Tensor currents. Similarly to the Dirac equation, where we had a conserved current density vector field $j^\mu(x)$, we are now looking for *conserved tensor currents*.

Definition: For N particles and Minkowski spacetime, a *tensor current* is a collection of continuously differentiable maps $(\mu_1, ..., \mu_N = 0, 1, 2, 3)$

$$j^{\mu_1 \cdots \mu_N} : \Omega \subset \mathbb{M}^N \to \mathbb{R}, \quad (x_1, ..., x_N) \to j^{\mu_1 \cdots \mu_N}(x_1, ..., x_N). \tag{5.33}$$

It is called *conserved if for all* $k = 1, ..., N$*:*

$$\partial_{x_k^{\mu_k}} j^{\mu_1 \cdots \mu_k \cdots \mu_N} = 0, \quad \mu_1, ..., \widehat{\mu_k}, ...\mu_N = 0, 1, 2, 3, \tag{5.34}$$

where $\widehat{(\cdot)}$ denotes omission.

Example. Let ψ be a C^1 solution of the free multi-time Dirac equations $(i\gamma_k^\mu \partial_{k,\mu} - m_k)\psi = 0$, $k = 1, ..., N$. Then

$$j^{\mu_1 \cdots \mu_N}(x_1, ..., x_N) = \overline{\psi}(x_1, ..., x_N)\gamma_1^{\mu_1} \cdots \gamma_N^{\mu_N} \psi(x_1, ..., x_N) \tag{5.35}$$

defines a conserved tensor current on $\mathbb{M}^N$ (see **Sheet 11, Exercise 1**).

For independent particles, the wave function is a tensor product of N single-particle wave functions $\psi_k : \mathbb{M} \to \mathbb{C}^4$ which all solve the Dirac equation, i.e.:

$$\psi(x_1, ..., x_N) = \psi_1(x_1) \otimes \cdots \otimes \psi_N(x_N). \tag{5.36}$$

For such a wave function, the Dirac tensor current (5.35) becomes:

$$j^{\mu_1 \cdots \mu_N}(x_1, ..., x_N) = j_1^{\mu_1}(x_1) \cdots j_N^{\mu_N}(x_N), \tag{5.37}$$

where $j_k^{\mu_k}(x_k) = \overline{\psi}_k(x_k)\gamma^\mu \psi_k(x_k)$. That means, it becomes the product of N single-particle Dirac currents.

As a consequence of the behavior of ψ under Lorentz transformations Λ (see Eq. (5.10)), the Dirac tensor current transforms as

$$j'^{\mu_1 \cdots \mu_N}(x_1', ..., x_N') = \Lambda^{\mu_1}{}_{\nu_1} \cdots \Lambda^{\mu_N}{}_{\nu_N} j^{\nu_1 \cdots \nu_N}(x_1, ..., x_N). \tag{5.38}$$

Given appropriate properties, the idea is to define a probability density via the tensor current. An important property such that this works is the following.

Definition: A tensor current j is called *positive definite* if for all $x_1, ..., x_N \in \mathbb{M}$ and all future-pointing time-like vectors $n_1, ..., n_N \in \mathbb{M}$:

$$j^{\mu_1 \cdots \mu_N}(x_1, ..., x_N)\, n_{\mu_1} \cdots n_{\mu_N} \geq 0 \tag{5.39}$$

and equality implies $j(x_1, ..., x_N) = 0$.

Definition: Let j be a positive definite and conserved tensor current and Σ be a space-like hyperplane (or more generally a smooth Cauchy surface) with future-pointing unit normal vector field n. Then we call the non-negative function defined by

$$\rho_\Sigma(x_1, ..., x_N) = j^{\mu_1 \cdots \mu_N}(x_1, ..., x_N)\, n_{\mu_1}(x_1) \cdots n_{\mu_N}(x_N) \tag{5.40}$$

the *density* of j with respect to Σ.

Remark. This definition generalizes the usual notion of a probability density in a natural way. For example, for the Dirac tensor current (5.35) we have:

(i) For $N = 1$, $\rho_\Sigma(x) = j^\mu(x) n_\mu(x)$ reduces to the familiar probability density with respect to Σ.

(ii) For $N \geq 2$ and an equal-time hyperplane Σ_t in a certain frame, we have $n(x) = (1,0,0,0)$ and thus $\rho_{\Sigma_t}(t, \mathbf{x}_1, ..., t, \mathbf{x}_N) = (\psi^\dagger \psi)(t, \mathbf{x}_1, ..., t, \mathbf{x}_N) = (\varphi^\dagger \varphi)(t, \mathbf{x}_1, ..., \mathbf{x}_N)$. So the density ρ_Σ reduces to the usual single-time probability density in that case (as expected).

In general, one can integrate ρ_Σ over arbitrary subsets of a space-like hyperplane (smooth Cauchy surface). Together with the above, this suggests:

Generalized Born rule. Let $\Sigma \subset \mathbb{M}$ be a space-like hyperplane (smooth Cauchy surface) and ρ_Σ the associated density. Furthermore, assume that ρ_Σ is normalized in the sense

$$\int_\Sigma d\sigma(x_1) \cdots \int_\Sigma d\sigma(x_N)\, \rho_\Sigma(x_1, ..., x_N) = 1. \tag{5.41}$$

Then, the *generalized Born rule* is the statement that

$$\text{Prob}(x_1 \in d\sigma(x_1), ..., x_N \in d\sigma(x_N)) = \rho_\Sigma(x_1, ..., x_N) d\sigma(x_1) \cdots d\sigma(x_N) \tag{5.42}$$

is the probability to detect N particles, each particle i in the infinitesimal 3-volume $d\sigma(x_i)$ around $x_i \in \Sigma$, $i = 1, ..., N$.

Important remark. The generalized Born rule can actually be shown, in an appropriate sense, to follow *as a theorem* from the Born rule in just one frame (i.e. at equal times). The proof can be found in the work

- M. Lienert and R. Tumulka, *Born's rule for arbitrary Cauchy surfaces,* `https://arxiv.org/abs/1706.07074`.

The idea is that in principle, the results of any experiment can also be obtained at a later equal time, and thus they should be determined already by the Born rule in one frame. However, it is not immediately clear that the result should be *a simple expression in the multi-time wave function* such as (5.42), and it is, in fact, quite some effort to demonstrate this.

Total probability conservation. Matching with the generalized Born rule, we have the following theorem:

Theorem 5.3.1 *Let j be a conserved tensor current on $\mathbb{M}^N$ which has compact support in the spatial directions, i.e. there is an $R > 0$ such that if there is a $k \in \mathbb{N}$ with $1 \leq k \leq N$ such that $|\mathbf{x}_k| > R$, we have $j(t_1, \mathbf{x}_1, ..., t_N, \mathbf{x}_N) = 0$. Let Σ, Σ' be space-like hyperplanes (smooth Cauchy surfaces) and let*

$$P(\Sigma) = \int_\Sigma d\sigma(x_1) \cdots \int_\Sigma d\sigma(x_N)\, \rho_\Sigma(x_1, ..., x_N). \tag{5.43}$$

Then we have $P(\Sigma) = P(\Sigma')$.

The proof is similar to the one of **Sheet 11, Exercise 1 (c)**.

Current density form. In many physical applications, it is more realistic to have a multi-time wave function (and consequently a tensor current) defined only on a subset $\Omega \subset \mathbb{R}^{4N}$, such as on the space-like configurations $\mathscr{S}$ (5.13). Then total probability conservation amounts to $P_\Omega(\Sigma) = P_\Omega(\Sigma')$ for all space-like hyperplanes (smooth Cauchy surfaces) Σ, Σ' where

$$P_\Omega(\Sigma) = \int_\Sigma d\sigma(x_1) \cdots \int_\Sigma d\sigma(x_N)\, \mathbb{1}_\Omega(x_1, ..., x_N)\, \rho_\Sigma(x_1, ..., x_N). \tag{5.44}$$

Here, $\mathbb{1}_\Omega$ is the characteristic function of Ω, i.e., $\mathbb{1}_\Omega(q) = 1$ if $q \in \Omega$ and 0 else.

In order to prove probability conservation in this sense, it is useful to express the statement in a different mathematical language, using an appropriately defined differential form which can be integrated along the relevant sets $\Sigma^N \cap \Omega$. (The main reason why this becomes necessary is to be able to use Stoke's theorem applied to these sets instead of the divergence theorem applied to each Σ factor-wise in the case of $\Omega = \mathbb{M}^N$.)

Definition: Let j be a tensor current on $\Omega \subset \mathbb{R}^{(1+d)N}$ on the relativistic configuration space $\mathbb{R}^{(1+d)N}$ for $1+d$-dimensional spacetime. Furthermore, let j have compact support in the spatial directions (as explained above). Then we define a Nd-form, the *current density form* ω_j, by

$$\begin{aligned}\omega_j = \sum_{\mu_1,...,\mu_N=0}^{d} (-1)^{\mu_1+\cdots+\mu_N} j^{\mu_1\cdots\mu_N}\, dx_1^0 \wedge \cdots \wedge \widehat{dx_1^{\mu_1}} \wedge \cdots \wedge dx_1^d \\ \wedge \cdots \wedge dx_N^0 \wedge \cdots \wedge \widehat{dx_N^{\mu_N}} \wedge \cdots \wedge dx_N^d,\end{aligned} \tag{5.45}$$

where $\widehat{(\cdot)}$ denotes omission.

Lemma 5.3.2 *The probability integral* (5.44) *can be expressed by*

$$P_\Omega(\Sigma) = \int_{\Sigma^N \cap \Omega} \omega_j. \tag{5.46}$$

Proof: This follows from the identity

$$n_\mu\, d\sigma = (-1)^\mu\, dx^0 \wedge \cdots \wedge \widehat{dx^\mu} \wedge \cdots \wedge dx^d. \tag{5.47}$$

→ **Sheet 12, Exercise 2.**

Lemma 5.3.3 *The exterior derivative of* ω_j *vanishes,* $d\omega_j = 0$.

Proof: Sheet 12, Exercise 2.

Remark. The current density form ω_j is useful as one can use Stokes' theorem for it. This becomes necessary to prove probability conservation for the model we shall discuss next.

5.4 An interacting multi-time model in 1+1 dimensions

In the following we show that it is possible to construct an interacting and completely Lorentz invariant multi-time model.[6] To this end, we choose the simplest possible case:

1. $N = 2$ Dirac particles,
2. only one ($d = 1$) spatial dimension,
3. massless particles.

The interactions will be so-called *contact interactions*, i.e., interactions which are associated with boundary conditions for the wave function at configurations (x, x) where two particles meet.

Defining equations. As mentioned above and as studied further on **Sheet 11, Exercise 2**, the most natural domain for a multi-time wave function is the set $\mathscr{S}$ of space-like configurations. In 1+1 dimensions, this set splits into two disjoint open sets,

$$\begin{aligned} \mathscr{S}_1 &= \{(t_1, z_1, t_2, z_2) \in \mathscr{S} : z_1 < z_2\}, \\ \mathscr{S}_2 &= \{(t_1, z_1, t_2, z_2) \in \mathscr{S} : z_1 > z_2\}. \end{aligned} \tag{5.48}$$

We shall construct a model on $\mathscr{S}_1$. Once a solution is found, it can then be extended to $\mathscr{S}_2$ by applying a reflection.

The multi-time wave function then is a map

$$\psi : \overline{\mathscr{S}}_1 \subset \mathbb{R}^2 \times \mathbb{R}^2 \to \mathbb{C}^4, \quad (t_1, z_1, t_2, z_2) \mapsto \psi(t_1, z_1, t_2, z_2). \tag{5.49}$$

On the open set $\mathscr{S}_1$, it obeys the free multi-time Dirac equations with $m_1 = m_2 = 0$:

$$i\gamma_k^\mu \partial_{k,\mu} \psi(x_1, x_2) = 0, \quad k = 1, 2. \tag{5.50}$$

In the representation

$$\gamma^0 = \sigma^1, \quad \gamma^1 = \sigma^1 \sigma^3, \tag{5.51}$$

(5.50) becomes diagonal:

$$\begin{aligned} \partial_{t_1} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} &= -\partial_{z_1} \begin{pmatrix} 1 & & & \\ & 1 & & \\ & & -1 & \\ & & & -1 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}, \\ \partial_{t_2} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} &= -\partial_{z_2} \begin{pmatrix} 1 & & & \\ & -1 & & \\ & & 1 & \\ & & & -1 \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}. \end{aligned} \tag{5.52}$$

[6] This section follows M. Lienert, *A relativistically interacting exactly solvable multi-time model for two mass-less Dirac particles in 1+1 dimensions*, J. Math. Phys. 56, 042301 (2015).

This means, the general solution of (5.50) is given by

$$\begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix}(t_1, z_1, t_2, z_2) = \begin{pmatrix} f_1(z_1 - t_1, z_2 - t_2) \\ f_2(z_1 - t_1, z_2 + t_2) \\ f_3(z_1 + t_1, z_2 - t_2) \\ f_4(z_1 + t_1, z_2 + t_2) \end{pmatrix}, \tag{5.53}$$

where f_1, f_2, f_3, f_4 are (still unkown) C^1 functions. They have to be determined by initial and boundary conditions.

Initial conditions are, as usual, given for $t_1, t_2 = 0$:

$$\psi(0, z_1, 0, z_2) = g(z_1, z_2) \text{ for } z_1 \leq z_2, \tag{5.54}$$

where $g \in C^1(\mathbb{R}^2, \mathbb{C}^4)$.

In addition, we will see that boundary conditions at

$$\mathscr{C} = \{(t_1, z_1, t_2, z_2) \in \mathbb{R}^2 \times \mathbb{R}^2 : t_1 = t_2 \text{ and } z_1 = z_2\} \subset \partial\mathscr{S}_1 \tag{5.55}$$

are necessary to ensure total probability conservation in the sense $P_{\mathscr{S}_1}(\Sigma) = P_{\mathscr{S}_1}(\Sigma')$ for all space-like hyperplanes Σ, Σ' (or smooth Cauchy surfaces, see (5.44) for the definition of $P_\Omega(\Sigma)$). Probability conservation is, in turn, related to the uniqueness of solutions, as follows from the energy integral technique applied to $P_{\mathscr{S}_1}(\Sigma)$.

Indeed, we can see from (5.53) that initial data determine the functions $f_i(x, y)$ only for $x \leq y$, namely through $f_i(x, y) = g_i(x, y)$, $x < y$, $i = 1, 2, 3, 4$. However, in $\mathscr{S}_1$, the quantities $x = z_1 - t_1$ and $y = z_2 + t_2$ which occur in the argument of f_2 can, for example, also have the relation $x > y$, for example for $t_1 = t_2 = t$ with $t < (z_1 - z_2)/2 < 0$. As the respective spacetime configuration (t_1, z_1, t_2, z_2) lies in in $\mathscr{S}_1$ (at equal times, the only restriction is $z_1 < z_2$), ψ_2 is not fully determined by initial data. The situation is similar for ψ_3 (there, ψ_3 may not be determined by intial data for example for $t_1 = t_2 = t$ with $t > (z_2 - z_1)/2 > 0$). For ψ_1, ψ_4 no such problem occurs, as for $i = 1, 4$ the quantities a_i, b_i in $f_i(a_i, b_i)$ in formula (5.53) always satisfy $a_i < b_i$ for $(t_1, z_1, t_2, z_2) \in \mathscr{S}_1$.

It will be the role of the boundary conditions to determine the missing values of the f_i, $i = 2, 3$.

Boundary conditions from probability conservation. On $\mathscr{S}_1$, the Dirac tensor current

$$j^{\mu\nu} = \overline{\psi}\gamma_1^\mu\gamma_2^\nu\psi \tag{5.56}$$

satisfies $\partial_{1,\mu}j^{\mu\nu} = 0 = \partial_{2,\nu}j^{\mu\nu}$ (as can be shown as in the case of free multi-time Dirac equations).

The idea now is to look for conditions on $j^{\mu\nu}$ which also ensure total probability conservation. These will then yield the appropriate boundary conditions.

Theorem 5.4.1 *Let $\psi : \overline{\mathscr{S}}_1 \to \mathbb{C}^4$ be a C^1-solution of (5.50) with compact spatial support for all fixed times $t_1, t_2 \in \mathbb{R}$. Moreover, let $j^{\mu\nu} : \overline{\mathscr{S}}_1 \to \mathbb{R}$ with $j^{\mu\nu} = \overline{\psi}\gamma_1^\mu\gamma_2^\nu\psi$ be the Dirac current constructed from ψ. Then*

$$P_{\mathscr{S}_1}(\Sigma) = P_{\mathscr{S}_1}(\Sigma') \tag{5.57}$$

holds for all space-like hyperplanes (Cauchy surfaces) $\Sigma, \Sigma' \subset \mathbb{M}$ *if the following condition for the tensor current is satisfied:*

$$(j^{01} - j^{10})(t, z, t, z) = 0 \ \forall t, z \in \mathbb{R}. \tag{5.58}$$

Proof: Sheet 12, Exercise 2 (using the theorem of Stokes for the current density form ω_j and for an appropriately chosen closed surface).

Remark. (5.58) has the meaning that there is no probability flux through the set of coincidence points $\mathscr{C}$. This means that there is no probability flux from $\mathscr{S}_1$ to $\mathscr{S}_2$, or in other words: the two particles cannot pass each other.

Our next task is to convert this condition into a boundary condition for ψ.

Lemma 5.4.2 *Condition* (5.58) *is equivalent to the following linear boundary condition for* ψ *on* $\mathscr{C}$*:*

$$\psi_2(t, z, t, z) = e^{i\theta(t,z)} \psi_3(t, z, t, z) \ \forall t, z \in \mathbb{R} \tag{5.59}$$

and some function $\theta(t, z)$*.*

Proof: Writing out the tensor current in components gives:

$$j^{\mu\nu} = |\psi_1|^2 + (-1)^\nu |\psi_2|^2 + (-1)^\mu |\psi_3|^2 + (-1)^\mu (-1)^\nu |\psi_4|^2. \tag{5.60}$$

Thus:

$$\begin{aligned} j^{01} - j^{10} &= (|\psi_1|^2 - |\psi_2|^2 + |\psi_3|^2 - |\psi_4|^2) - (|\psi_1|^2 + |\psi_2|^2 - |\psi_3|^2 - |\psi_4|^2) \\ &= 2(|\psi_3|^2 - |\psi_2|^2). \end{aligned} \tag{5.61}$$

Therefore,

$$\begin{aligned} & j^{01} - j^{10} = 0 \\ \Leftrightarrow \quad & |\psi_2| = |\psi_3| \\ \Leftrightarrow \quad & \psi_2 = e^{i\theta} \psi_3. \end{aligned} \tag{5.62}$$

for a function $\theta : \mathbb{R}^2 \to [0, 2\pi)$. The claim follows. □

As we aim for a translation invariant model, we choose $\theta = \text{const}$.

Theorem 5.4.3 *Let* $\theta \in [0, 2\pi)$*. Then multi-time model defined by* (5.49), (5.50) *on* $\mathscr{S}_1$*, initial conditions* (5.54) *and boundary conditions*

$$\psi_2(q) = e^{i\theta} \psi_3(q), \quad q \in \mathscr{C} \tag{5.63}$$

has a unique solution given by

$$\begin{aligned} \psi_1(t_1, z_1, t_2, z_2) &= g_1(z_1 - t_1, z_2 - t_2), \\ \psi_2(t_1, z_1, t_2, z_2) &= \begin{cases} g_2(z_1 - t_1, z_2 + t_2) & \text{for } z_1 - t_1 < z_2 + t_2, \\ e^{i\theta} g_3(z_2 + t_2, z_1 - t_1) & \text{for } z_1 - t_1 \geq z_2 + t_2, \end{cases} \\ \psi_3(t_1, z_1, t_2, z_2) &= \begin{cases} g_3(z_1 + t_1, z_2 - t_2) & \text{for } z_1 + t_1 < z_2 - t_2, \\ e^{-i\theta} g_2(z_2 - t_2, z_1 + t_1) & \text{for } z_1 + t_1 \geq z_2 - t_2, \end{cases} \\ \psi_4(t_1, z_1, t_2, z_2) &= g_4(z_1 + t_1, z_2 + t_2). \end{aligned} \tag{5.64}$$

This solution is continuously differentiable provided $g \in C^1(\mathbb{R}^2, \mathbb{C}^4)$ *satisfies the following compatibility conditions between boundary values and initial data: for all* $z \in \mathbb{R}$*:*

1. $g_2(z,z) = e^{i\theta} g_3(z,z)$,
2. $(\partial_1 g_2)(z,z) = e^{i\theta}(\partial_2 g_3)(z,z)$,
3. $(\partial_2 g_2)(z,z) = e^{i\theta}(\partial_1 g_3)(z,z)$.

Condition 1 ensures continuity of ψ, conditions 2 and 3 guarantee continuous differentiability.

Proof: The fact that (5.64) is a solution of the IBVP can be shown by direct computation. Condition 1 is needed so that the initial data satisfy the boundary condition, and furthermore for continuity of ψ at the critial surfaces $z_1 - t_1 = z_2 + t_2$ and $z_1 + t_1 + z_2 - t_2$. Conditions 2 and 3 are necessary so that the different limits of the partial derivatives of ψ towards these critical surfaces are continuous. Uniqueness can either be shown using the form of the general solution (5.53) or through the energy integral technique applied to $P_{\mathscr{S}_1}(\Sigma)$. → **Sheet 13, Exercise 1.**

Idea behind the solution formula. The above proof does of course not explain how to come up with the solution formula. The idea behind it is the following. The general solution formula (5.53) shows that each component ψ_i of the solution is constant along certain two dimensional surfaces in $\mathbb{R}^2 \times \mathbb{R}^2$. For ψ_1, for example, these surfaces are given by $z_1 - z_2 = \text{const}_1$, $z_2 - t_2 = \text{const}_2$. Thus, if one wants to know the value of ψ_1 at a point $p = (t_1, z_1, t_2, z_2) \in \mathscr{S}_1$, one checks if the surface going through p intersects the initial data surface $t_1 = t_2 = 0$. This is always the case but the point q where this happens (it is actually a point, not a line!) may not lie in $\mathscr{S}_1$. For ψ_1 it always does, and we have $q = (0, z_1 - t_1, z_2 - t_2)$. Then $\psi_1(p) = \psi_1(q) = g_1(z_1 - t_1, z_2 - t_2)$. The situation is similar for ψ_4. For f_2 and f_3, however, the analogously defined point q sometimes does not lie in $\mathscr{S}_1$. Then one instead checks whether the surface along which ψ_i, $i \in \{2,3\}$ is constant intersects the boundary $\mathscr{C}$. This indeed happens in a point $r \in \mathscr{C}$. Then the value of, say, $\psi_2(p)$ is obtained through the boundary condition as $\psi_2(p) = \psi_2(r) = e^{i\theta}\psi_3(r)$. This is only a known quantity if $\psi_3(r)$ is known. However, one can check that at each $s \in \mathscr{C}$ either $\psi_2(s)$ or $\psi_3(s)$ is determined by initial data. Thus, this way of determining ψ_2 and ψ_3 completely always works. For more details see the paper J. Math. Phys. 56, 042301 (2015), also available under `https://arxiv.org/abs/1411.2833`.

Interaction. Why is the model interacting? Well, a model is called interacting if it is not free, and free means that all initial product wave function stay product wave functions with the time evolution. Thus "interacting" means that there are initial product wave functions which do not stay product wave functions for all times. We can see from the solution formula (5.64) that this is the case for our model by letting $g(z_1, z_2) = g_a(z_1) \otimes g_b(z_2)$ for two functions $g_a, g_b \in C^1(\mathbb{R}, \mathbb{C}^2)$. The product structure is not always preserved, as one can see from the case differentiations in the formulas for ψ_2, ψ_3.

One calls such a type of interaction which is achieved through boundary conditions on the coincidence points *contact interactions*, or *zero-range* or *delta-interactions*. Such interactions are related to delta function potentials in the Hamiltonian of a

single-time theory. These delta function potentials are not mathematically well-defined but one can understand them rigorously by integrating over the Schrödinger equation and thus extracting a boundary condition. Then the regular part of the Hamiltonian together with this boundary condition define the dynamics.

Lorentz invariance. We have not yet checked the Lorentz invariance of the model. For the multi-time equations, this is clear, as the Dirac equation and the domain $\mathscr{S}_1$ are Lorentz invariant. However, it is not yet clear whether also the boundary conditions are Lorentz invariant. To check this, we need to know how a Lorentz transformation acts on ψ. Let $\Lambda \in \mathcal{L}_+^\uparrow$. Then, according to (5.10), we have:

$$\psi'(t_1', z_1', t_2', z_2') = S[\Lambda] \otimes S[\Lambda]\, \psi(t_1, z_1, t_2, z_2). \tag{5.65}$$

For $(t_1, z_1, t_2, z_2) \in \mathscr{C}$, we also have $(t_1', z_1', t_2', z_2') \in \mathscr{C}$, so the Lorentz transform of the boundary condition (5.63) is again a boundary condition on $\mathscr{C}$. The question however, remains, whether this boundary condition is of the same form as (5.63).

To see this in detail, we note that the Lorentz group in 1+1 dimensions has just one generator, the generator of boosts in z-direction. Thus, according to (4.60), $S[\Lambda]$ is given by:

$$S[\Lambda] = \exp(\omega\, \gamma^0\gamma^1/2) \tag{5.66}$$

for some $\omega \in \mathbb{R}$. Here, we have $\gamma^0\gamma^1 = \sigma^3$ which is diagonal. Thus,

$$S[\Lambda] = \cosh(\omega/2)\, \mathbb{1}_2 + \sinh(\omega/2)\, \sigma^3. \tag{5.67}$$

It follows that

$$S[\Lambda]\otimes S[\Lambda] = \cosh^2(\omega/2)\, \mathbb{1}_4 + \cosh(\omega/2)\sinh(\omega/2)(\mathbb{1}_2\otimes\sigma^3 + \sigma^3\otimes\mathbb{1}_2) + \sinh^2(\omega/2)\sigma^3\otimes\sigma_3. \tag{5.68}$$

Explicitly, considering

$$(\mathbb{1}_2 \otimes \sigma^3 + \sigma^3 \otimes \mathbb{1}_2) = 2\,\mathrm{diag}(1, 0, 0, -1), \quad \sigma^3 \otimes \sigma^3 = \mathrm{diag}(1, -1, -1, 1), \tag{5.69}$$

this means that

$$\begin{aligned} S[\Lambda] \otimes S[\Lambda] \begin{pmatrix} \psi_1 \\ \psi_2 \\ \psi_3 \\ \psi_4 \end{pmatrix} &= \begin{pmatrix} (\cosh(\omega/2) + \sinh(\omega/2))^2\psi_1 \\ (\cosh^2(\omega/2) - \sinh^2(\omega/2))\psi_2 \\ (\cosh^2(\omega/2) - \sinh^2(\omega/2))\psi_3 \\ (\cosh(\omega/2) - \sinh(\omega/2))^2 \end{pmatrix} \\ &= \begin{pmatrix} (\cosh(\omega/2) + \sinh(\omega/2))^2\psi_1 \\ \psi_2 \\ \psi_3 \\ (\cosh(\omega/2) - \sinh(\omega/2))^2\psi_4 \end{pmatrix}. \end{aligned} \tag{5.70}$$

So the components ψ_2, ψ_3 transform without any factor. Accordingly, the boundary condition (5.63) transforms to

$$\psi_2'(t', z', t', z') = e^{i\theta}\psi_3'(t', z', t', z'), \tag{5.71}$$

which is again a boundary condition of the form (5.63). Thus, it is indeed Lorentz invariant.

As one can also choose initial data on any space-like hyperplane (this can be shown similarly to **Sheet 5, Exercise 3**), the model is overall Lorentz invariant. Probability conservation also holds on all space-like hyperplanes (and, accordingly, in all Lorentz frames).

Summary. Overall, we have shown that it is possible to achieve Lorentz invariant interacting dynamics for multi-time wave functions.