

# Appendix A:

## Lagrangian Mechanics

Lagrangian mechanics is not only a very beautiful and powerful formulation of mechanics, but it is also needed as a preparation for a deeper understanding of all fundamental interactions in physics. All fundamental equations of motion in physics are encoded in Lagrangian field theory, which is a generalization of Lagrangian mechanics for fields. Furthermore, the connection between symmetries and conservation laws of physical systems is best explored in the framework of the Lagrangian formulation of dynamics, and we also need Lagrangian field theory as a basis for field quantization.

Suppose we consider a particle with coordinates  $\mathbf{x}(t)$  moving in a potential  $V(\mathbf{x})$ . Then Newton's equation of motion

$$m\ddot{\mathbf{x}} = -\nabla V(\mathbf{x})$$

is equivalent to the following statement (Hamilton's principle, 1834): The action integral

$$S[\mathbf{x}] = \int_{t_0}^{t_1} dt L(\mathbf{x}, \dot{\mathbf{x}}) = \int_{t_0}^{t_1} dt \left( \frac{m}{2} \dot{\mathbf{x}}^2 - V(\mathbf{x}) \right)$$

is in first order stationary under arbitrary perturbations  $\mathbf{x}(t) \rightarrow \mathbf{x}(t) + \delta\mathbf{x}(t)$  of the path of the particle between fixed endpoints  $\mathbf{x}(t_0)$  and  $\mathbf{x}(t_1)$  (i.e. the perturbation is only restricted by the requirement of fixed endpoints:  $\delta\mathbf{x}(t_0) = 0$  and  $\delta\mathbf{x}(t_1) = 0$ ). This is demonstrated by straightforward calculation of the first order variation of  $S$ ,

$$\begin{aligned} \delta S[\mathbf{x}] &= S[\mathbf{x} + \delta\mathbf{x}] - S[\mathbf{x}] = \int_{t_0}^{t_1} dt [m\dot{\mathbf{x}} \cdot \delta\dot{\mathbf{x}} - \delta\mathbf{x} \cdot \nabla V(\mathbf{x})] \\ &= - \int_{t_0}^{t_1} dt \delta\mathbf{x} \cdot (m\ddot{\mathbf{x}} + \nabla V(\mathbf{x})). \end{aligned} \tag{A.1}$$

Partial integration and  $\delta\mathbf{x}(t_0) = 0$ ,  $\delta\mathbf{x}(t_1) = 0$  were used in the last step. Equation (A.1) tells us that  $\delta S[\mathbf{x}] = 0$  holds for arbitrary path variation with fixed endpoints if and only if the path  $\mathbf{x}(t)$  satisfies Newton's equations,

$$m\ddot{\mathbf{x}} + \nabla V(\mathbf{x}) = 0.$$

This generalizes to arbitrary numbers of particles ( $\mathbf{x}(t) \rightarrow \mathbf{x}_I(t)$ ,  $1 \leq I \leq N$ ), and to the case that the motion of the particles is restricted through constraints, like e.g. a particle that can only move on a sphere<sup>1</sup>. In the case of constraints one substitutes generalized coordinates  $q_i(t)$  which correspond to the actual degrees of freedom of the particle or system of particles (e.g. polar angles for the particle on the sphere), and one ends up with an action integral of the form

$$S[q] = \int_{t_0}^{t_1} dt L(q, \dot{q}).$$

The function  $L(q, \dot{q})$  is the *Lagrange function* of the mechanical system with generalized coordinates  $q_i(t)$ , and a shorthand notation is used for a mechanical system with  $N$  degrees of freedom,

$$(q, \dot{q}) = (q_1(t), q_2(t), \dots, q_N(t), \dot{q}_1(t), \dot{q}_2(t), \dots, \dot{q}_N(t)).$$

First order variation of the action with fixed endpoints (i.e.  $\delta q(t_0) = 0$ ,  $\delta q(t_1) = 0$ ) yields after partial integration

$$\begin{aligned} \delta S[q] &= S[q + \delta q] - S[q] = \int_{t_0}^{t_1} dt \left( \sum_i \delta q_i \frac{\partial L}{\partial q_i} + \sum_i \delta \dot{q}_i \frac{\partial L}{\partial \dot{q}_i} \right) \\ &= \int_{t_0}^{t_1} dt \sum_i \delta q_i \left( \frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} \right), \end{aligned} \quad (\text{A.2})$$

where again fixation of the endpoints was used.

$\delta S[q] = 0$  for arbitrary path variation  $q_i(t) \rightarrow q_i(t) + \delta q_i(t)$  with fixed endpoints then immediately tells us the equations of motion in terms of the generalized coordinates,

$$\frac{\partial L}{\partial q_i} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_i} = 0. \quad (\text{A.3})$$

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<sup>1</sup>And it also applies to relativistic particles, see Appendix B.

These equations of motion are called Lagrange equations of the second kind or Euler-Lagrange equations or simply Lagrange equations. The quantity

$$p_i = \frac{\partial L}{\partial \dot{q}_i}$$

is denoted as the *conjugate momentum* to the coordinate  $q_i$ .

The conjugate momentum is conserved if the Lagrange function depends only on the generalized velocity component  $\dot{q}_i$  but not on  $q_i$ ,  $dp_i/dt = 0$ .

Furthermore, if the Lagrange function does not explicitly depend on time, we have

$$\frac{dL}{dt} = p_i \ddot{q}_i + \frac{\partial L}{\partial q_i} \dot{q}_i.$$

The Euler-Lagrange equation then implies that the Hamilton function

$$H = p_i \dot{q}_i - L$$

is conserved,  $dH/dt = 0$ .

For a simple example, consider a particle of mass  $m$  in a gravitational field  $\mathbf{g} = -g\mathbf{e}_z$ . The particle is constrained so that it can only move on a sphere of radius  $r$ . An example of generalized coordinates are angles  $\vartheta$ ,  $\varphi$  on the sphere, and the Cartesian coordinates  $\{X, Y, Z\}$  of the particle are related to the generalized coordinates through

$$X(t) = r \sin \vartheta(t) \cdot \cos \varphi(t),$$

$$Y(t) = r \sin \vartheta(t) \cdot \sin \varphi(t),$$

$$Z(t) = r \cos \vartheta(t).$$

The kinetic energy of the particle can be expressed in terms of the generalized coordinates,

$$K = \frac{m}{2} \dot{\mathbf{r}}^2 = \frac{m}{2} (\dot{X}^2 + \dot{Y}^2 + \dot{Z}^2) = \frac{m}{2} r^2 (\dot{\vartheta}^2 + \dot{\varphi}^2 \sin^2 \vartheta),$$

and the potential energy is

$$V = mgZ = mgr \cos \vartheta.$$

This yields the Lagrange function in the generalized coordinates,

$$L = \frac{m}{2} \dot{\mathbf{r}}^2 - mgZ = \frac{m}{2} r^2 (\dot{\vartheta}^2 + \dot{\varphi}^2 \sin^2 \vartheta) - mgr \cos \vartheta,$$

and the Euler-Lagrange equations yield the equations of motion of the particle,

$$\ddot{\vartheta} = \dot{\varphi}^2 \sin \vartheta \cos \vartheta + \frac{g}{r} \sin \vartheta, \quad (\text{A.4})$$

$$\frac{d}{dt} (\dot{\varphi} \sin^2 \vartheta) = 0. \quad (\text{A.5})$$

The conjugate momenta

$$p_{\vartheta} = \frac{\partial L}{\partial \dot{\vartheta}} = mr^2 \dot{\vartheta}$$

and

$$p_{\varphi} = \frac{\partial L}{\partial \dot{\varphi}} = mr^2 \dot{\varphi} \sin^2 \vartheta$$

are just the angular momenta for rotation in  $\vartheta$  or  $\varphi$  direction. The Hamilton function is the conserved energy

$$H = p_{\vartheta} \dot{\vartheta} + p_{\varphi} \dot{\varphi} - L = \frac{p_{\vartheta}^2}{2mr^2} + \frac{p_{\varphi}^2}{2mr^2 \sin^2 \vartheta} + mgr \cos \vartheta = K + U.$$

The immediately apparent advantage of this formalism is that it directly yields the correct equations of motion (A.4, A.5) for the system without ever having to worry about finding the force that keeps the particle on the sphere. Beyond that the formalism also provides a systematic way to identify conservation laws in mechanical systems, and if one actually wants to know the force that keeps the particle on the sphere (which is actually trivial here, but more complicated e.g. for a system of two particles which have to maintain constant distance), a simple extension of the formalism to the Lagrange equations of the first kind can yield that, too.

The Lagrange function is not simply the difference between kinetic and potential energy if the forces are velocity dependent. This is the case for the Lorentz force. The Lagrange function for a non-relativistic charged particle in electromagnetic fields is

$$L = \frac{m}{2} \dot{\mathbf{x}}^2 + q\dot{\mathbf{x}} \cdot \mathbf{A} - q\Phi.$$

This yields the correct Lorentz force law  $m\ddot{\mathbf{x}} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B})$  for the particle, cf. Section 15.1. The relativistic versions of the Lagrange function for the particle can be found in equations (B.24, B.25).

## Direct derivation of the Euler-Lagrange equations for the generalized coordinates $q_a$ from Newton's equation in Cartesian coordinates

We can derive the Euler-Lagrange equations for the generalized coordinates of a constrained  $N$ -particle system directly from Newton's equations. This works in the following way:

Suppose we have  $N$  particles with coordinates  $x_i^j$ ,  $1 \leq i \leq N$ ,  $1 \leq j \leq 3$ , moving in a potential  $V(\mathbf{x}_{1\dots N})$ . The Newton equations

$$\frac{d}{dt}(m_i \dot{x}_i^j) + \frac{\partial}{\partial x_i^j} V(\mathbf{x}_{1\dots N}) = 0$$

can be written as

$$\left( \frac{d}{dt} \frac{\partial}{\partial \dot{x}_i^j} - \frac{\partial}{\partial x_i^j} \right) \left( \frac{1}{2} \sum_k m_k \dot{x}_k^2 - V(\mathbf{x}_{1\dots N}) \right) = 0, \quad (\text{A.6})$$

or equivalently

$$\left( \frac{d}{dt} \frac{\partial}{\partial \dot{x}_i^j} - \frac{\partial}{\partial x_i^j} \right) L(\mathbf{x}_{1\dots N}, \dot{\mathbf{x}}_{1\dots N}) = 0, \quad (\text{A.7})$$

with the Lagrange function

$$L(\mathbf{x}_{1\dots N}, \dot{\mathbf{x}}_{1\dots N}) = \frac{1}{2} \sum_i m_i \dot{x}_i^2 - V(\mathbf{x}_{1\dots N}). \quad (\text{A.8})$$

If there are  $C$  holonomic constraints on the motion of the  $N$ -particle system, we can describe its trajectories through  $3N - C$  generalized coordinates  $q_a$ ,  $1 \leq a \leq 3N - C$ :

$$x_i^j = x_i^j(q, t). \quad (\text{A.9})$$

Note that in general  $x_i^j(q, t)$  will implicitly depend on time  $t$  through the time dependence of the generalized coordinates  $q_a(t)$ , but it may also explicitly depend on  $t$  because there may be a time dependence in the  $C$  constraints<sup>2</sup>.

The velocity components of the system are

$$\dot{x}_i^j = \frac{dx_i^j}{dt} = \sum_a \dot{q}_a \frac{\partial x_i^j}{\partial q_a} + \frac{\partial x_i^j}{\partial t}. \quad (\text{A.10})$$

<sup>2</sup>A simple example for the latter would e.g. be a particle that is bound to a sphere with radius  $R(t)$ , where  $R(t)$  is a given time-dependent function.

This implies in particular the equations

$$\frac{\partial \dot{x}_i^j}{\partial \dot{q}_a} = \frac{\partial x_i^j}{\partial q_a} \quad (\text{A.11})$$

and

$$\frac{\partial \dot{x}_i^j}{\partial q_a} = \sum_b \dot{q}_b \frac{\partial^2 x_i^j}{\partial q_a \partial q_b} + \frac{\partial^2 x_i^j}{\partial t \partial q_a}. \quad (\text{A.12})$$

Substitution of (A.11) into (A.12) yields

$$\frac{\partial \dot{x}_i^j}{\partial q_a} = \sum_b \dot{q}_b \frac{\partial^2 \dot{x}_i^j}{\partial q_b \partial \dot{q}_a} + \frac{\partial^2 \dot{x}_i^j}{\partial t \partial \dot{q}_a}. \quad (\text{A.13})$$

Equation (A.11) also yields

$$\frac{\partial^2 \dot{x}_i^j}{\partial \dot{q}_a \partial \dot{q}_b} = 0,$$

and this implies with (A.13)

$$\frac{d}{dt} \frac{\partial \dot{x}_i^j}{\partial \dot{q}_a} = \sum_b \dot{q}_b \frac{\partial^2 \dot{x}_i^j}{\partial q_b \partial \dot{q}_a} + \frac{\partial^2 \dot{x}_i^j}{\partial t \partial \dot{q}_a} = \frac{\partial \dot{x}_i^j}{\partial q_a}. \quad (\text{A.14})$$

With these preliminaries we can now look at the following linear combinations of the Newton equations (A.7):

$$\sum_{i,j} \frac{\partial x_i^j}{\partial q_a} \cdot \left( \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_i^j} - \frac{\partial L}{\partial x_i^j} \right) = 0.$$

Insertion of equations (A.11, A.14) yields

$$\sum_{i,j} \left[ \frac{\partial \dot{x}_i^j}{\partial \dot{q}_a} \frac{d}{dt} \frac{\partial L}{\partial \dot{x}_i^j} - \frac{\partial x_i^j}{\partial q_a} \frac{\partial L}{\partial x_i^j} + \left( \frac{d}{dt} \frac{\partial \dot{x}_i^j}{\partial \dot{q}_a} - \frac{\partial \dot{x}_i^j}{\partial q_a} \right) \frac{\partial L}{\partial \dot{x}_i^j} \right] = 0,$$

or after combining terms:

$$\frac{d}{dt} \sum_{i,j} \left( \frac{\partial \dot{x}_i^j}{\partial \dot{q}_a} \frac{\partial L}{\partial \dot{x}_i^j} \right) - \frac{\partial L}{\partial q_a} = 0. \quad (\text{A.15})$$

However, the coordinates  $x_i^j$  are independent of the generalized velocities  $\dot{q}_a$ , and therefore equation (A.15) is just the Lagrange equation (A.3):

$$\frac{d}{dt} \frac{\partial L(q, \dot{q})}{\partial \dot{q}_a} - \frac{\partial L(q, \dot{q})}{\partial q_a} = 0. \quad (\text{A.16})$$

## Symmetries and conservation laws in classical mechanics

We call a set of first order transformations

$$t \rightarrow t' = t - \epsilon(t), \quad q_a(t) \rightarrow q'_a(t') = q_a(t) + \delta q_a(t) \quad (\text{A.17})$$

a symmetry of a mechanical system with action

$$S[q] = \int_{t_0}^{t_1} dt L(q(t), \dot{q}(t), t)$$

if it changes the form  $dt L(q(t), \dot{q}(t), t)$  in first order of  $\epsilon(t)$  and  $\delta q_a(t)$  at most by a term of the form  $dB = dt(dB/dt)$ :

$$\begin{aligned} \delta(dt L(q, \dot{q}, t)) &\equiv dt' L(q'(t'), \dot{q}'(t'), t') - dt L(q(t), \dot{q}(t), t) \\ &= dt \frac{d}{dt} B_{\delta q, \epsilon}(q(t), t). \end{aligned} \quad (\text{A.18})$$

To see how this implies conservation laws in the mechanical system, we have to evaluate  $\delta(dt L(q, \dot{q}, t))$  for the transformations (A.17). We have to take into account that (A.17) implies

$$dt' = dt(1 - \dot{\epsilon}(t)), \quad \frac{d}{dt'} = (1 + \dot{\epsilon}(t)) \frac{d}{dt},$$

and therefore also

$$\delta \dot{q}_a(t) = \frac{d}{dt'} q'_a(t') - \frac{d}{dt} q_a(t) = \dot{\epsilon}(t) \frac{d}{dt} q_a(t) + \frac{d}{dt} \delta q_a(t).$$

The first order change in  $dt L$  is therefore

$$\begin{aligned} \delta(dt L) &= dt' L(q'(t'), \dot{q}'(t'), t') - dt L(q(t), \dot{q}(t), t) \\ &= dt \left[ \delta q_a \frac{\partial L}{\partial q_a} + \left( \dot{\epsilon} \frac{d}{dt} q_a + \frac{d}{dt} \delta q_a \right) \frac{\partial L}{\partial \dot{q}_a} - \dot{\epsilon} L - \epsilon \frac{\partial L}{\partial t} \right]. \end{aligned}$$

Now we substitute

$$\delta\dot{q}_a \frac{\partial L}{\partial \dot{q}_a} = \frac{d}{dt} \left( \delta q_a \frac{\partial L}{\partial \dot{q}_a} \right) - \delta q_a \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_a}$$

and

$$\begin{aligned} \dot{\epsilon} \left( \dot{q}_a \frac{\partial L}{\partial \dot{q}_a} - L \right) &= \frac{d}{dt} \left( \epsilon \dot{q}_a \frac{\partial L}{\partial \dot{q}_a} - \epsilon L \right) - \epsilon \ddot{q}_a \frac{\partial L}{\partial \dot{q}_a} - \epsilon \dot{q}_a \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_a} + \epsilon \frac{dL}{dt} \\ &= \frac{d}{dt} \left( \epsilon \dot{q}_a \frac{\partial L}{\partial \dot{q}_a} - \epsilon L \right) + \epsilon \dot{q}_a \left( \frac{\partial L}{\partial q_a} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_a} \right) + \epsilon \frac{\partial L}{\partial t}. \end{aligned}$$

This yields

$$\begin{aligned} \delta(dtL) &= dt (\delta q_a + \epsilon \dot{q}_a) \left( \frac{\partial L}{\partial q_a} - \frac{d}{dt} \frac{\partial L}{\partial \dot{q}_a} \right) \\ &\quad + dt \frac{d}{dt} \left( (\delta q_a + \epsilon \dot{q}_a) \frac{\partial L}{\partial \dot{q}_a} - \epsilon L \right). \end{aligned} \quad (\text{A.19})$$

Comparison of equations (A.18) and (A.19) implies an on-shell conservation law

$$\frac{d}{dt} Q_{\delta q, \epsilon} = 0$$

with the conserved charge

$$Q_{\delta q, \epsilon} = \epsilon \left( L - \dot{q}_a \frac{\partial L}{\partial \dot{q}_a} \right) - \delta q_a \frac{\partial L}{\partial \dot{q}_a} + B_{\delta q, \epsilon}. \quad (\text{A.20})$$

$B_{\delta q, \epsilon}$  is the one-dimensional version of the current  $K^\mu$  in Lagrangian field theory and  $Q_{\delta q, \epsilon}$  is the one-dimensional version of the conserved current  $J^\mu$ , see the paragraph after equation (16.14).  $B_{\delta q, \epsilon} = 0$  in most cases. However, a noticeable exception are Galilei boosts in nonrelativistic  $N$ -particle mechanics (where  $I$  enumerates the particles). The Lagrange function

$$L = \frac{1}{2} m_I \dot{\mathbf{x}}_I^2 - V_{I < J}(|\mathbf{x}_I - \mathbf{x}_J|) \quad (\text{A.21})$$

satisfies (A.18) for Galilei transformations  $\epsilon(t) = 0$ ,  $\delta \mathbf{x}_I(t) = -\mathbf{v}t$ . In this case  $B = -m_I \mathbf{x}_I(t) \cdot \mathbf{v}$  and the conservation law

$$Q = m_I \mathbf{v} \cdot [\dot{\mathbf{x}}_I(t)t - \mathbf{x}_I(t)] = \mathbf{v} \cdot [\mathbf{P}t - M\mathbf{X}(t)]$$

assures uniform center of mass motion  $\mathbf{X}(t)$  with velocity  $\mathbf{P}/M$ . Other familiar symmetry transformations of (A.21) include time translations  $\epsilon(t) = \text{const.}$ , which yields energy conservation,

$$H = -Q/\epsilon = \dot{\mathbf{x}}_I \cdot \frac{\partial L}{\partial \dot{\mathbf{x}}_I} - L = \frac{1}{2} m_I \dot{\mathbf{x}}_I^2 + V_{I < J}(|\mathbf{x}_I - \mathbf{x}_J|),$$

spatial translations  $\delta \mathbf{x}_I(t) = \boldsymbol{\epsilon} = \text{const.}$ , which yields conservation of total momentum,

$$\mathbf{P} = -\frac{\partial Q}{\partial \boldsymbol{\epsilon}} = m_I \dot{\mathbf{x}}_I,$$

and rotations  $\delta \mathbf{x}_I(t) = \boldsymbol{\varphi} \times \mathbf{x}_I(t)$ , which yields conservation of total angular momentum,

$$\mathbf{M} = -\frac{\partial Q}{\partial \boldsymbol{\varphi}} = m_I \mathbf{x}_I \times \dot{\mathbf{x}}_I.$$

The corresponding conserved charges from the symmetries of the Lagrange function  $L = -mc\sqrt{c^2 - \dot{\mathbf{x}}^2(t)}$  of a free relativistic particle are

$$\mathbf{p} = \frac{\partial L}{\partial \dot{\mathbf{x}}} = \frac{m\dot{\mathbf{x}}}{\sqrt{1 - (\dot{\mathbf{x}}/c)^2}},$$

$$H = cp^0 = \dot{\mathbf{x}} \cdot \mathbf{p} - L = \frac{mc^2}{\sqrt{1 - (\dot{\mathbf{x}}/c)^2}} = c\sqrt{\mathbf{p}^2 + m^2c^2},$$

$$\mathbf{M} = \mathbf{x} \times \mathbf{p},$$

and the conserved charges which follow from Lorentz invariance  $\delta x^\mu = \omega^{\mu\nu} x_\nu$ ,  $\omega^{\mu\nu} = -\omega^{\nu\mu}$ , are

$$M^{\mu\nu} = x^\mu p^\nu - x^\nu p^\mu,$$

which of course includes the charges  $L_i = \epsilon_{ijk} M^{jk}/2$  from rotations. See also Appendix B.

# Appendix B: The Covariant Formulation of Electrodynamics

Electrodynamics is a relativistic field theory for every frequency or energy of electromagnetic waves because photons are massless. Understanding of electromagnetism and of photon-matter interactions therefore requires an understanding of special relativity. Furthermore, we also want to understand the quantum mechanics of relativistic electrons and other relativistic particles, and the covariant formulation of electrodynamics is also very helpful as a preparation for relativistic wave equations like the Klein-Gordon and Dirac equations.

## Lorentz transformations

The scientific community faced several puzzling problems around 1900. Some of these problems led to the development of quantum mechanics, but two of the problems motivated Einstein's Special Theory of Relativity:

- In 1881 and 1887 Michelson had demonstrated that light from a terrestrial light source always moves with the same speed  $c$  in each direction, irrespective of Earth's motion.
- The basic equation of Newtonian mechanics,  $\mathbf{F} = d(\mathbf{mu})/dt$ , is invariant under Galilei transformations of the coordinates:

$$t' = t, \quad \mathbf{x}' = \mathbf{x} - \mathbf{v}t. \tag{B.1}$$

Therefore any two observers who use coordinates related through a Galilei transformation are physically equivalent in Newtonian mechanics.

However, in 1887 (at the latest) it was realized that Galilei transformations do not leave Maxwell's equations invariant, i.e. if Maxwell's equations describe electromagnetic phenomena for one observer, they would not hold for another observer

moving with constant velocity  $\mathbf{v}$  relative to the first observer (because it was assumed that the coordinates of these two observers are related through the Galilei transformation (B.1)). Instead, Voigt (1887) and Lorentz (1892–1904) realized that Maxwell's equations would hold for the two observers if their coordinates would be related e.g. through a transformation of the form

$$ct' = \frac{ct - (v/c)x}{\sqrt{1 - (v^2/c^2)}}, \quad x' = \frac{x - vt}{\sqrt{1 - (v^2/c^2)}}, \quad y' = y, \quad z' = z, \quad (\text{B.2})$$

and they also realized that coordinate transformations of this kind imply that light would move with the same speed  $c$  in both coordinate systems,

$$\Delta x^2 + \Delta y^2 + \Delta z^2 - c^2 \Delta t^2 = \Delta x'^2 + \Delta y'^2 + \Delta z'^2 - c^2 \Delta t'^2. \quad (\text{B.3})$$

Voigt was interested in the most general symmetry transformation of the wave equations for electromagnetic fields, while Lorentz tried to explain the results of the Michelson experiment.

In 1905 Einstein took the bold step to propose that then the coordinates measured by two observers with constant relative speed  $v$  must be described by transformations like (B.2), but *not* by Galilei transformations<sup>1</sup>. This was a radical step, because it implies that two observers with non-vanishing relative speed assign different time coordinates to one and the same event, and they also have different notions of simultaneity of events. The same statement in another formulation: Two different observers with non-vanishing relative speed slice the four-dimensional universe differently into three-dimensional regions of simultaneity, or into three-dimensional universes. Einstein abandoned the common prejudice that everybody always assigns the same time coordinate to one and the same event. Time is not universal. The speed of light in vacuum is universal.

In the following we use the abbreviations

$$\beta = \frac{v}{c}, \quad \gamma = \frac{1}{\sqrt{1 - \beta^2}}.$$

The transformation (B.2) and its inversion then read

$$ct' = \gamma(ct - \beta x), \quad x' = \gamma(x - \beta ct), \quad y' = y, \quad z' = z, \quad (\text{B.4})$$

$$ct = \gamma(ct' + \beta x'), \quad x = \gamma(x' + \beta ct'). \quad (\text{B.5})$$

The spatial origin  $x' = y' = z' = 0$  of the  $(ct', x', y', z')$  system satisfies  $x = \beta ct = vt$  (use  $x' = 0$  in  $x' = \gamma(x - \beta ct)$ ), and therefore moves with velocity  $v\mathbf{e}_x$

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<sup>1</sup>This idea was also enunciated by Poincaré in 1904, but Einstein went beyond the statement of the idea and also worked out the consequences.

relative to the  $(ct, x, y, z)$  system. In the same way one finds that the spatial origin of the  $(ct, x, y, z)$  system moves with velocity  $-v\mathbf{e}'_x$  through the  $(ct', x', y', z')$  system. Therefore this is the special Lorentz transformation between two coordinate frames with a relative motion with speed  $v$  in  $x$ -direction as seen from the unprimed frame, or in  $(-x')$ -direction as seen from the primed frame.

Equation (B.2) tells us that for motion in a certain direction ( $x$ -direction in (B.2)), the coordinate in that direction is affected non-trivially by the transformation, while any orthogonal coordinate does not change its value. This immediately allows for a generalization of (B.2) in the case that the relative velocity  $\mathbf{v}$  points in an arbitrary direction.

It is convenient to introduce a rescaled velocity vector  $\boldsymbol{\beta} \equiv \mathbf{v}/c$  and the corresponding unit vector  $\hat{\boldsymbol{\beta}} = \boldsymbol{\beta}/\beta = \mathbf{v}/v$ . The  $(3 \times 3)$ -matrix  $\hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T$  projects any vector  $\mathbf{x}$  onto its component parallel to  $\boldsymbol{\beta}$ ,

$$\mathbf{x}_{\parallel\boldsymbol{\beta}} = \hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T \cdot \mathbf{x},$$

while the component orthogonal to  $\boldsymbol{\beta}$  is

$$\mathbf{x}_{\perp\boldsymbol{\beta}} = \mathbf{x} - \mathbf{x}_{\parallel\boldsymbol{\beta}} = (\mathbf{1} - \hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T) \cdot \mathbf{x}.$$

From the form of the special Lorentz transformation (B.2) we know that the coordinate  $|\mathbf{x}_{\parallel\boldsymbol{\beta}}|$  parallel to  $\mathbf{v}$  will be rescaled by a factor

$$\gamma = \frac{1}{\sqrt{1 - (v^2/c^2)}} = \frac{1}{\sqrt{1 - \beta^2}},$$

and be shifted by an amount  $-\gamma vt = -\gamma\boldsymbol{\beta}ct$ . Similarly, the time coordinate  $ct$  will be rescaled by the factor  $\gamma$  and be shifted by an amount  $-\gamma\boldsymbol{\beta}|\mathbf{x}_{\parallel\boldsymbol{\beta}}|$ . Finally, nothing will happen to the transverse component  $\mathbf{x}_{\perp\boldsymbol{\beta}}$ . We can collect these observations in a  $(4 \times 4)$ -matrix equation relating the two four-dimensional coordinate vectors,

$$\begin{pmatrix} ct' \\ \mathbf{x}' \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma\boldsymbol{\beta}^T \\ -\gamma\boldsymbol{\beta} & \mathbf{1} - \hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T + \gamma\hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T \end{pmatrix} \cdot \begin{pmatrix} ct \\ \mathbf{x} \end{pmatrix}$$

This is the general Lorentz transformation between two observers if the spatial sections of their coordinate frames were coincident at  $t = 0$ . The most general transformation of this kind also allows for constant shifts of the coordinates and for a rotation of the spatial axes,

$$\begin{pmatrix} ct' \\ \mathbf{x}' \end{pmatrix} = \begin{pmatrix} \gamma & -\gamma\boldsymbol{\beta}^T \\ -\gamma\boldsymbol{\beta} & \mathbf{1} - \hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T + \gamma\hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T \end{pmatrix} \cdot \begin{pmatrix} \mathbf{1} & \mathbf{0}^T \\ \mathbf{0} & \underline{R} \end{pmatrix} \cdot \begin{pmatrix} ct - cT \\ \mathbf{x} - \mathbf{X} \end{pmatrix}, \quad (\text{B.6})$$

where  $\underline{R}$  is a  $3 \times 3$  rotation matrix. Without the coordinate shifts this is the most general orthochronous Lorentz transformation, where *orthochronous* refers to the

fact that we did not include a possible reversal of the time axis. With the coordinate shifts included, (B.6) is denoted as an inhomogeneous Lorentz transformation or a Poincaré transformation. The Poincaré transformations (B.6) and the subset of Lorentz transformations ( $T = 0$ ,  $\mathbf{X} = \mathbf{0}$ ) form the *Poincaré group* and the *Lorentz group*, respectively. The Lorentz group is apparently a subgroup of the Poincaré group, and the rotation group is a subgroup of the Lorentz group.

In four-dimensional notation the 4-vector of coordinates is  $x^\mu = (ct, \mathbf{x})$ , and the 4-vector short hand for equation (B.6) is

$$x'^\mu = \Lambda^\mu{}_\nu (x^\nu - X^\nu). \quad (\text{B.7})$$

where the  $(4 \times 4)$  transformation matrix  $\Lambda$  is

$$\Lambda = \{\Lambda^\mu{}_\nu\} = \begin{pmatrix} \gamma & & -\gamma\boldsymbol{\beta}^T \\ -\gamma\boldsymbol{\beta} & \underline{1} - \hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T + \gamma\hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T \end{pmatrix} \cdot \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \underline{R} \end{pmatrix}. \quad (\text{B.8})$$

A homogeneous Lorentz transformation of this form is denoted as a *proper orthochronous Lorentz transformation* if we also exclude inversions of an odd number of spatial axis<sup>2</sup>. This is equivalent to the requirement  $\det \underline{R} = 1$ .

We will see below that it plays a role where we attach the indices for the explicit numerical representation of the matrix  $\Lambda$  in terms of matrix elements. Usually, if a matrix is given for  $\Lambda$  without explicitly defining index positions, the default convention is that it refers to a superscript row index and a subscript column index, as above,  $\Lambda = \{\Lambda^\mu{}_\nu\}$ . This is important, because as soon as a boost is involved (i.e.  $\boldsymbol{\beta} \neq \mathbf{0}$ ), we will find that e.g.

$$\Lambda^\mu{}_\nu(\boldsymbol{\beta}) = \Lambda_\nu{}^\mu(-\boldsymbol{\beta}) \neq \Lambda_\nu{}^\mu(\boldsymbol{\beta}).$$

The transformation equation (B.6) is the general solution to the following problem: Find the most general coordinate transformation  $\{ct, \mathbf{x}\} = \{ct, x, y, z\} \rightarrow \{ct', \mathbf{x}'\} = \{ct', x', y', z'\}$  which leaves the expression  $\Delta \mathbf{x}^2 - c^2 \Delta t^2$  invariant, i.e. such that for arbitrary coordinate differentials  $c \Delta t$ ,  $\Delta \mathbf{x}$  we have

$$\Delta \mathbf{x}^2 - c^2 \Delta t^2 = \Delta \mathbf{x}'^2 - c^2 \Delta t'^2. \quad (\text{B.9})$$

This equation implies in particular that if one of our observers sees a light wave moving at speed  $c$ , then this light wave will also move with speed  $c$  for the second observer,

$$\Delta \mathbf{x}^2 - c^2 \Delta t^2 = 0 \Leftrightarrow \Delta \mathbf{x}'^2 - c^2 \Delta t'^2 = 0.$$

<sup>2</sup>The two factors of a proper orthochronous Lorentz transformation can be written as exponentials. This is discussed in Appendix H.

In fact it suffices to require *only* that anything moving with speed  $c$  will also have speed  $c$  in the new coordinates, and that the spatial coordinates are Cartesian in both frames. Up to rescalings of the coordinates the most general coordinate transformation is then the general inhomogeneous Lorentz transformation (B.6).

Any constant offset  $X^\mu$  between coordinate systems vanishes for differences of coordinates. Equation (B.7) therefore implies the following equation for Lorentz transformation of coordinate differentials,

$$dx'^\mu = \Lambda^\mu{}_\alpha dx^\alpha. \quad (\text{B.10})$$

The condition (B.9),

$$dx^2 - c^2 dt^2 = dx'^2 - c^2 dt'^2$$

can also be written as

$$\eta_{\mu\nu} dx'^\mu dx'^\nu = \eta_{\alpha\beta} dx^\alpha dx^\beta \quad (\text{B.11})$$

with the special  $(4 \times 4)$ -matrix ( $\underline{1}$  is the  $3 \times 3$  unit matrix)

$$\eta_{\mu\nu} = \begin{pmatrix} -1 & \mathbf{0}^T \\ \mathbf{0} & \underline{1} \end{pmatrix},$$

Equation (B.9) also implies

$$\eta_{\mu\nu} dx'^\mu dy'^\nu = \eta_{\alpha\beta} dx^\alpha dy^\beta$$

for any pair of Lorentz transformed 4-vectors  $dx$  and  $dy$  (simply insert the 4-vector  $dx + dy$  into (B.11)). This implies that Lorentz transformations leave the *Minkowski metric*  $\eta_{\mu\nu}$  invariant:

$$\eta_{\mu\nu} \Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta = \eta_{\alpha\beta}. \quad (\text{B.12})$$

If we multiply this equation with the components  $\eta^{\beta\gamma}$  of the inverse Minkowski tensor, we find

$$\eta_{\mu\nu} \Lambda^\mu{}_\alpha \Lambda^\nu{}_\beta \eta^{\beta\gamma} = \delta_\alpha{}^\gamma \equiv \eta_\alpha{}^\gamma.$$

This tells us a relation between the  $(4 \times 4)$ -matrix  $\Lambda$  with “pulled indices” and its inverse  $\Lambda^{-1}$ :

$$\Lambda_\mu{}^\gamma \equiv \eta_{\mu\nu} \Lambda^\nu{}_\beta \eta^{\beta\gamma} = (\Lambda^{-1})^\gamma{}_\mu. \quad (\text{B.13})$$

Explicitly, if

$$\{\Lambda^{\mu}_{\nu}\} = \begin{pmatrix} \gamma & -\gamma\boldsymbol{\beta}^T \\ -\gamma\boldsymbol{\beta} & \mathbb{1} - \hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T + \gamma\hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T \end{pmatrix} \cdot \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \underline{R} \end{pmatrix}$$

then

$$\{\Lambda_{\mu}^{\nu}\} \equiv \{\eta_{\mu\rho}\Lambda^{\rho}_{\sigma}\eta^{\sigma\nu}\} = \begin{pmatrix} \gamma & \gamma\boldsymbol{\beta}^T \\ \gamma\boldsymbol{\beta} & \mathbb{1} - \hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T + \gamma\hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T \end{pmatrix} \cdot \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \underline{R} \end{pmatrix}.$$

We can also “pull” or “draw” indices on 4-vectors, e.g.  $dx_{\alpha} \equiv \eta_{\alpha\beta}dx^{\beta} = (-cdt, dx)$ . Let us figure out how this 4-vector transforms under the Lorentz transformation (B.10):

$$dx'_{\mu} = \eta_{\mu\nu}dx'^{\nu} = \eta_{\mu\nu}\Lambda^{\nu}_{\alpha}dx^{\alpha} = \eta_{\mu\nu}\Lambda^{\nu}_{\alpha}\eta^{\alpha\beta}dx_{\beta} = \Lambda_{\mu}^{\beta}dx_{\beta} = dx_{\beta}(\Lambda^{-1})^{\beta}_{\mu}.$$

4-vectors with this kind of transformation behavior are denoted as *covariant 4-vectors*, while  $dx^{\mu}$  is an example of a *contravariant 4-vector*. Another example of a covariant 4-vector is the vector of partial derivatives

$$\partial_{\mu} \equiv \frac{\partial}{\partial x^{\mu}} = \left( \frac{1}{c} \frac{\partial}{\partial t}, \nabla \right).$$

We can check that this is really a covariant 4-vector by calculating how it transforms under Lorentz transformations. According to the chain rule of differentiation we find

$$\partial'_{\mu} \equiv \frac{\partial}{\partial x'^{\mu}} = \frac{\partial x^{\alpha}}{\partial x'^{\mu}} \frac{\partial}{\partial x^{\alpha}}.$$

However, we have

$$dx^{\alpha} = (\Lambda^{-1})^{\alpha}_{\nu} dx'^{\nu} \quad \Rightarrow \quad \frac{\partial x^{\alpha}}{\partial x'^{\mu}} = (\Lambda^{-1})^{\alpha}_{\mu}$$

and therefore

$$\partial'_{\mu} = (\Lambda^{-1})^{\alpha}_{\mu} \partial_{\alpha} = \Lambda_{\mu}^{\alpha} \partial_{\alpha}.$$

Pairs of co- and contravariant indices do not transform if they are summed over. Assume e.g. that  $F^{\alpha\beta}$  are the components of a  $4 \times 4$  matrix which transform according to

$$F^{\alpha\beta} \rightarrow F'^{\mu\nu} = \Lambda^{\mu}_{\alpha} \Lambda^{\nu}_{\beta} F^{\alpha\beta}.$$

The combination  $\partial_{\alpha} F^{\alpha\beta}$  then transforms under Lorentz transformations according to

$$\partial'_{\mu} F'^{\mu\nu} = \Lambda_{\mu}^{\alpha} \partial_{\alpha} \Lambda^{\mu}_{\beta} \Lambda^{\nu}_{\gamma} F^{\beta\gamma} = \Lambda^{\nu}_{\gamma} \eta^{\alpha}_{\beta} \partial_{\alpha} F^{\beta\gamma} = \Lambda^{\nu}_{\gamma} \partial_{\alpha} F^{\alpha\gamma},$$

i.e. the summed index pair does not contribute to the transformation. Only “free” indices (i.e. indices which are not paired and summed from 0 to 3) transform under Lorentz transformations.

### The manifestly covariant formulation of electrodynamics

Electrodynamics is a Lorentz invariant theory, i.e. all equations have the same form in all coordinate systems which are related by Poincaré transformations. However, this property is hardly recognizable if one looks at Maxwell’s equations in traditional notation,

$$\begin{aligned} \nabla \cdot \mathbf{E} &= \frac{1}{\epsilon_0} \rho, & \nabla \times \mathbf{E} + \frac{\partial}{\partial t} \mathbf{B} &= \mathbf{0}, \\ \nabla \cdot \mathbf{B} &= 0, & \nabla \times \mathbf{B} - \frac{1}{c^2} \frac{\partial}{\partial t} \mathbf{E} &= \mu_0 \mathbf{j}. \end{aligned}$$

“Lorentz invariance” seems far from obvious: How, e.g. would the electric and magnetic fields transform under a Lorentz transformation of the coordinates? Apparently we seem to have three 3-dimensional vectors and one scalar in the equations. We can combine the current density  $\mathbf{j}$  and the charge density  $\rho$  into a current 4-vector

$$j^\nu = (\rho c, \mathbf{j}).$$

For the field strengths it helps to recall that the homogeneous Maxwell’s equations are solved through potentials  $\Phi, \mathbf{A}$ ,

$$\mathbf{B} = \nabla \times \mathbf{A}, \quad \mathbf{E} = -\frac{\partial}{\partial t} \mathbf{A} - \nabla \Phi.$$

If one combines the potentials into a 4-vector,

$$A_\mu = (-\Phi/c, \mathbf{A}),$$

it is possible to realize that the electromagnetic field strengths  $E_i, B_i$  are related to antisymmetric combinations of the 4-vectors  $\partial_\mu, A_\nu$ ,

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu = \begin{pmatrix} 0 & -E_1/c & -E_2/c & -E_3/c \\ E_1/c & 0 & B_3 & -B_2 \\ E_2/c & -B_3 & 0 & B_1 \\ E_3/c & B_2 & -B_1 & 0 \end{pmatrix}. \tag{B.14}$$

This electromagnetic field strength tensor  $\underline{F}$  was introduced by Minkowski in 1907<sup>3</sup>. The matrix elements  $F_{\mu\nu}$  are its covariant components. The contravariant components of  $\underline{F}$  are

$$F^{\mu\nu} = \eta^{\mu\alpha} \eta^{\nu\beta} F_{\alpha\beta} = \partial^\mu A^\nu - \partial^\nu A^\mu = \begin{pmatrix} 0 & E_1/c & E_2/c & E_3/c \\ -E_1/c & 0 & B_3 & -B_2 \\ -E_2/c & -B_3 & 0 & B_1 \\ -E_3/c & B_2 & -B_1 & 0 \end{pmatrix}.$$

From this one can easily read off the transformation behavior of the fields under Lorentz transformations,

$$\begin{aligned} x^\mu &\rightarrow x'^\mu = \Lambda^\mu{}_\alpha x^\alpha, \\ \partial_\mu &\rightarrow \partial'_\mu = \Lambda_\mu{}^\alpha \partial_\alpha, \\ A_\mu(x) &\rightarrow A'_\mu(x') = \Lambda_\mu{}^\alpha A_\alpha(x) \end{aligned}$$

$$\begin{aligned} F_{\mu\nu}(x) &\rightarrow F'_{\mu\nu}(x') = \partial'_\mu A'_\nu(x') - \partial'_\nu A'_\mu(x') = \Lambda_\mu{}^\alpha \Lambda_\nu{}^\beta (\partial_\alpha A_\beta(x) - \partial_\beta A_\alpha(x)) \\ &= \Lambda_\mu{}^\alpha \Lambda_\nu{}^\beta F_{\alpha\beta}(x). \end{aligned}$$

Evaluation of  $F'_{\mu\nu}(x')$  for a boost

$$\{\Lambda^\mu{}_\nu\} = \begin{pmatrix} \gamma & & & -\gamma \boldsymbol{\beta}^T \\ -\gamma \boldsymbol{\beta} & \mathbb{1} - \hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T + \gamma \hat{\boldsymbol{\beta}} \otimes \hat{\boldsymbol{\beta}}^T \end{pmatrix}$$

yields with  $\boldsymbol{\beta} = \mathbf{v}/c$

$$\begin{aligned} \mathbf{E}'(x', t') &= \gamma \left( \mathbf{E}(\mathbf{x}, t) + \mathbf{v} \times \mathbf{B}(\mathbf{x}, t) \right) - (\gamma - 1) \hat{\boldsymbol{\beta}} \left( \hat{\boldsymbol{\beta}} \cdot \mathbf{E}(\mathbf{x}, t) \right) \\ &= \gamma \left( \mathbf{E}(\mathbf{x}, t) + \mathbf{v} \times \mathbf{B}(\mathbf{x}, t) \right) - \frac{\gamma^2}{(\gamma + 1)c^2} \mathbf{v} \left( \mathbf{v} \cdot \mathbf{E}(\mathbf{x}, t) \right), \\ \mathbf{B}'(x', t') &= \gamma \left( \mathbf{B}(\mathbf{x}, t) - \frac{1}{c^2} \mathbf{v} \times \mathbf{E}(\mathbf{x}, t) \right) - (\gamma - 1) \hat{\boldsymbol{\beta}} \left( \hat{\boldsymbol{\beta}} \cdot \mathbf{B}(\mathbf{x}, t) \right) \\ &= \gamma \left( \mathbf{B}(\mathbf{x}, t) - \frac{1}{c^2} \mathbf{v} \times \mathbf{E}(\mathbf{x}, t) \right) - \frac{\gamma^2}{(\gamma + 1)c^2} \mathbf{v} \left( \mathbf{v} \cdot \mathbf{B}(\mathbf{x}, t) \right), \end{aligned}$$

<sup>3</sup>H. Minkowski, Math. Ann. 68, 472 (1910). A translation of his results for dielectric materials into contemporary tensor notation can be found in R. Dick, Annalen Phys. (Berlin) 18, 174 (2009).

or expressed in terms of the field strength components parallel and perpendicular to the relative velocity  $\mathbf{v}$  between the two observers,

$$\begin{aligned} \mathbf{E}'_{\parallel}(\mathbf{x}', t') &= \mathbf{E}_{\parallel}(\mathbf{x}, t), & \mathbf{B}'_{\parallel}(\mathbf{x}', t') &= \mathbf{B}_{\parallel}(\mathbf{x}, t), \\ \mathbf{E}'_{\perp}(\mathbf{x}', t') &= \gamma \left( \mathbf{E}_{\perp}(\mathbf{x}, t) + \mathbf{v} \times \mathbf{B}_{\perp}(\mathbf{x}, t) \right), \\ \mathbf{B}'_{\perp}(\mathbf{x}', t') &= \gamma \left( \mathbf{B}_{\perp}(\mathbf{x}, t) - \frac{1}{c^2} \mathbf{v} \times \mathbf{E}_{\perp}(\mathbf{x}, t) \right). \end{aligned}$$

Electric and magnetic fields mix under Lorentz transformations, i.e. the distinction between electric and magnetic fields depends on the observer.

The equations

$$\partial_{\mu} F^{\mu\nu} = -\mu_0 \mathbf{j}^{\nu}$$

are the inhomogeneous Maxwell's equations

$$\nabla \cdot \mathbf{E} = \frac{1}{\epsilon_0} \rho, \quad \nabla \times \mathbf{B} - \frac{1}{c^2} \frac{\partial}{\partial t} \mathbf{E} = \mu_0 \mathbf{j},$$

while the identities (with the 4-dimensional  $\epsilon$ -tensor,  $\epsilon^{0123} = -1$ )

$$\epsilon^{\kappa\lambda\mu\nu} \partial_{\lambda} F_{\mu\nu} = 2\epsilon^{\kappa\lambda\mu\nu} \partial_{\lambda} \partial_{\mu} A_{\nu} \equiv 0$$

are the homogeneous Maxwell's equations

$$\nabla \cdot \mathbf{B} = 0, \quad \nabla \times \mathbf{E} + \frac{\partial}{\partial t} \mathbf{B} = \mathbf{0}.$$

These identities can also be written in terms of the dual field strength tensor

$$\tilde{F}^{\mu\nu} = \frac{1}{2} \epsilon^{\mu\nu\alpha\beta} F_{\alpha\beta} = \begin{pmatrix} 0 & -B_1 & -B_2 & -B_3 \\ B_1 & 0 & E_3/c & -E_2/c \\ B_2 & -E_3/c & 0 & E_1/c \\ B_3 & E_2/c & -E_1/c & 0 \end{pmatrix}$$

as

$$\partial_{\mu} \tilde{F}^{\mu\nu} = 0.$$

The gauge freedom  $A_{\mu}(x) \rightarrow A'_{\mu}(x) = A_{\mu}(x) + \partial_{\mu} f(x)$  apparently leaves the field strength tensor  $F_{\mu\nu}$  invariant. In conventional terms this is

$$\Phi'(x) = \Phi(x) - \dot{f}(x), \quad \mathbf{A}'(x) = \mathbf{A}(x) + \nabla f(x).$$

We have written Maxwell's equations explicitly as equations between 4-vectors,

$$\partial_\mu F^{\mu\nu} = -\mu_0 j^\nu, \quad \partial_\mu \tilde{F}^{\mu\nu} = 0,$$

and this ensures that they hold in this form for every inertial observer. This is the *form invariance* (or simply “invariance”) of Maxwell's equations under Lorentz transformations.

With the identification of the current 4-vector  $j^\mu = (\rho c, \mathbf{j})$ , the local conservation law for charges can also be written in manifestly Lorentz invariant form,

$$\frac{\partial}{\partial t} \rho + \nabla \cdot \mathbf{j} = \partial_\mu j^\mu = 0.$$

## Relativistic mechanics

In special relativity it is better to express everything in quantities which transform linearly with combinations of the matrices  $\Lambda$  and  $\Lambda^{-1}$ . As a consequence of the transformation law

$$dx'^\mu = \Lambda^\mu{}_\nu dx^\nu, \tag{B.15}$$

ordinary velocities  $d\mathbf{x}/dt$  and accelerations  $d^2\mathbf{x}/dt^2$  transform nonlinearly under Lorentz boosts, due to the transformation of the time coordinates in the denominators. Therefore it is convenient to substitute the physical velocities and accelerations with “proper” velocities and accelerations, which do not require division by a transforming time parameter  $t$ .

Suppose the  $x'$ -frame is the frame of a moving object. In its own frame the trajectory of the object is  $\mathbf{x}' = 0$ . However, we know that the Lorentz transformation (B.15) leaves the product  $dx^\mu dx_\mu$  invariant,

$$dx'^\mu dx'_\mu = dx'^2 - c^2 dt'^2 = dx^\mu dx_\mu = dx^2 - c^2 dt^2.$$

Therefore we have in particular for the time  $dt' \equiv d\tau$  measured by the moving object along its own path  $\mathbf{x}' = 0$

$$d\tau^2 = dt^2 - \frac{1}{c^2} dx^2 = \left(1 - \frac{v^2}{c^2}\right) dt^2,$$

i.e. up to a constant

$$\tau = \int dt \sqrt{1 - (v^2/c^2)} = \int \frac{dt}{\gamma}.$$

This is an *invariant*, i.e. it has the same value for each observer. Every observer will measure their own specific time interval  $\Delta t$  between any two events happening to the moving object, but all observers agree on the same value

$$\Delta\tau = \int_0^{\Delta t} dt \sqrt{1 - (v^2/c^2)}$$

which elapsed on a clock moving with the object.

The time  $\Delta\tau$  measured by an object between any two events happening to the object is denoted as the *proper time* or *eigentime* of the object.

The definition of eigentime entails a corresponding definition of the *proper velocity* or *eigenvelocity* of an object in an observer’s frame: Divide the change in the object’s coordinates  $d\mathbf{x}$  in the observer’s frame by the time interval  $d\tau$  elapsed for the object itself while it was moving by  $d\mathbf{x}$ :

$$\mathbf{U} = \frac{d\mathbf{x}}{d\tau} = \gamma \frac{d\mathbf{x}}{dt} = \gamma \mathbf{v}.$$

This is a hybrid construction in the sense that a set of coordinate intervals  $d\mathbf{x}$  measured in the observer’s frame is divided by a coordinate interval  $d\tau$  measured in the object’s frame<sup>4</sup>.

The notion of proper velocity may seem a little artificial, but it is useful because it can be extended to a 4-vector using the fact that  $\{dx^\mu\} = (dx^0, d\mathbf{x}) = (cdt, d\mathbf{x})$  is a 4-vector under Lorentz transformations. If we define

$$U^0 = \frac{dx^0}{d\tau} = \frac{cdt}{d\tau} = \gamma c,$$

then

$$U^\mu = dx^\mu/d\tau = (U^0, \mathbf{U}) = \gamma(c, \mathbf{v})$$

is a 4-vector which transforms according to  $U^\mu \rightarrow U'^\mu = \Lambda^\mu_\alpha U^\alpha$  under Lorentz transformations. This *4-velocity* vector satisfies

$$U^2 \equiv U^\mu U_\mu \equiv \eta_{\mu\nu} U^\mu U^\nu = \mathbf{U}^2 - (U^0)^2 = -c^2.$$

The conservation laws

$$\begin{aligned} \sum_i \mathbf{p}_i^{(in)} &= \sum_i \mathbf{p}_i^{(out)} \\ \sum_i E_i^{(in)} &= \sum_i E_i^{(out)} \end{aligned}$$

---

<sup>4</sup>There is a limit  $v \leq c$  on the *physical speed*  $v = |\mathbf{v}|$  of moving objects. No such limit holds for the “eigenspeed”  $|\mathbf{U}|$ , but the speed of signal transmission relative to an observer is  $v$ , not  $|\mathbf{U}|$ .

for momentum and energy in a collision would not be preserved under Lorentz transformations if the nonrelativistic definitions for momentum and energy would be employed, due to the nonlinear transformations of the particle velocities. This would mean that if momentum and energy conservation would hold for one observer, they would not hold for another observer with different velocity!

However, the conservation laws are preserved if energy and momentum transform linearly, like a 4-vector, under Lorentz transformations. We have already identified 4-velocities  $\{U^\mu\} = \gamma(c, \mathbf{v})$  with the property  $\lim_{\beta \rightarrow 0} \mathbf{U} = \mathbf{v}$ .

This motivates the definition of the *4-momentum*

$$p^0 = mU^0, \quad \mathbf{p} = m\mathbf{U},$$

i.e. the relativistic definition of the spatial momentum of a particle of mass  $m$  and physical velocity  $\mathbf{v}$  is

$$\mathbf{p} = m\mathbf{U} = \gamma m\mathbf{v} = \frac{m\mathbf{v}}{\sqrt{1 - (v^2/c^2)}}. \quad (\text{B.16})$$

The physical meaning of the fourth component

$$p^0 = mU^0 = \gamma mc = \frac{mc}{\sqrt{1 - (v^2/c^2)}}$$

can be inferred from the nonrelativistic limit:  $v \ll c$  yields

$$p^0 \simeq mc \left( 1 + \frac{v^2}{2c^2} \right).$$

This motivates the identification of  $cp^0$  with the energy of a particle of mass  $m$  and speed  $v$ :

$$E = cp^0 = \gamma mc^2 = \frac{mc^2}{\sqrt{1 - (v^2/c^2)}}. \quad (\text{B.17})$$

Division of the two equations (B.16) and (B.17) yields

$$\mathbf{v} = c^2 \frac{\mathbf{p}}{E}, \quad (\text{B.18})$$

and subtracting squares yields the relativistic dispersion relation

$$E^2 - c^2 \mathbf{p}^2 = m^2 c^4. \quad (\text{B.19})$$

This is usually written as  $p_\mu p^\mu = -m^2 c^2$ .

Equations (B.19) and (B.18) imply in particular for massless particles the relations  $E = cp$  and  $v = c$ .

For the formulation of the relativistic version of Newton's law, we observe that the rate of change of 4-momentum with eigentime defines a 4-vector with the units of force,

$$f^\mu = \frac{d}{d\tau} m \frac{dx^\mu}{d\tau} = \frac{dp^\mu}{d\tau} = \gamma \frac{d}{dt} p^\mu.$$

It transforms linearly under Lorentz transformations because we divided a 4-vector  $dx^\mu$  or  $dp^\mu$  by invariants  $d\tau^2$  or  $d\tau$ , respectively.

By convention one still defines three-dimensional forces according to

$$\mathbf{F} = \frac{d}{dt} \mathbf{p} = \frac{1}{\gamma} \mathbf{f},$$

i.e.  $\mathbf{F}$  is *not* the spatial component of a 4-vector, but  $\mathbf{f} = \gamma \mathbf{F}$  is.

For the 0-component  $f^0$  we find with the relativistic dispersion relation  $E = c\sqrt{\mathbf{p}^2 + m^2c^2}$ ,

$$\begin{aligned} f^0 &= \frac{d}{d\tau} m \frac{dx^0}{d\tau} = \frac{d}{d\tau} \left( m\gamma \frac{dx^0}{dt} \right) = \frac{d}{d\tau} (\gamma mc) = \frac{d}{d\tau} \frac{E}{c} = \frac{d}{d\tau} \sqrt{\mathbf{p}^2 + m^2c^2} \\ &= \frac{\mathbf{p}}{\sqrt{\mathbf{p}^2 + m^2c^2}} \cdot \frac{d}{d\tau} \mathbf{p} = \frac{\mathbf{v}}{c} \cdot \frac{d}{dt} \mathbf{p} = \frac{\mathbf{v}}{c} \cdot \mathbf{f}. \end{aligned} \tag{B.20}$$

The 4-vector of the force is therefore

$$(f^0, \mathbf{f}) = (\boldsymbol{\beta} \cdot \mathbf{f}, \mathbf{f}) = (\gamma \boldsymbol{\beta} \cdot \mathbf{F}, \gamma \mathbf{F}).$$

Multiplication of (cf. (B.20))

$$\frac{d}{d\tau} \frac{E}{c} = \frac{\mathbf{v}}{c} \cdot \mathbf{f}$$

with  $c/\gamma$  gives energy balance in conventional form,

$$\frac{d}{dt} E = \frac{c}{\sqrt{\mathbf{p}^2 + m^2c^2}} \mathbf{p} \cdot \frac{d}{dt} \mathbf{p} = \mathbf{v} \cdot \frac{d}{dt} \mathbf{p} = \mathbf{v} \cdot \mathbf{F}.$$

The nonrelativistic Newton equation for motion of a charged particle in electromagnetic fields contains the Lorentz force

$$\mathbf{F} = q\mathbf{E} + q\mathbf{v} \times \mathbf{B}.$$

We can get a hint at how the relativistic equation has to look like by expressing this combination of fields in terms of the field strength tensor (B.14),

$$E^i = cF^i_0 = F^i_0 \frac{dx^0}{dt}, \quad \varepsilon^i_{jk} B^k = F^i_j.$$

The latter equation implies

$$(\mathbf{v} \times \mathbf{B})^i = \varepsilon^i_{jk} v^j B^k = F^i_j v^j,$$

and therefore

$$F^i = qE^i + q\varepsilon^i_{jk} v^j B^k = qF^i_0 \frac{dx^0}{dt} + qF^i_j \frac{dx^j}{dt} = qF^i_\nu \frac{dx^\nu}{dt}.$$

This would be a spatial part of a 4-vector if we would not derive with respect to the laboratory time  $t$ , but with respect to the eigentime  $\tau$  of the charged particle:

$$f^i = \gamma F^i = qF^i_\nu \frac{dx^\nu}{d\tau}.$$

The time component is then

$$f^0 = qF^0_i \frac{dx^i}{d\tau} = q\gamma \frac{1}{c} E_i \frac{dx^i}{dt} = \gamma q \boldsymbol{\beta} \cdot \mathbf{E}$$

and the electromagnetic force 4-vector is

$$f^\mu = qF^\mu_\nu \frac{dx^\nu}{d\tau} = (\gamma q \boldsymbol{\beta} \cdot \mathbf{E}, \gamma q (\mathbf{E} + \mathbf{v} \times \mathbf{B})).$$

The equation of motion of the charged particle in 4-vector notation is therefore

$$m \frac{d^2 x^\mu}{d\tau^2} = qF^\mu_\nu \frac{dx^\nu}{d\tau},$$

or

$$m \ddot{x}^\mu(\tau) = qF^\mu_\nu(x(\tau)) \dot{x}^\nu(\tau). \quad (\text{B.21})$$

The time component yields after rescaling with  $c/\gamma$  again the energy balance equation

$$\frac{dE}{dt} = q\mathbf{v} \cdot \mathbf{E}. \quad (\text{B.22})$$

The spatial part is after rescaling with  $\gamma^{-1}$ :

$$\frac{d}{dt} \mathbf{p} = q(\mathbf{E} + \mathbf{v} \times \mathbf{B}). \quad (\text{B.23})$$

The only changes in (B.22, B.23) with respect to the nonrelativistic equations are the velocity dependences of  $E$  and  $\mathbf{p}$ :

$$\mathbf{p} = \frac{m\mathbf{v}}{\sqrt{1 - (v^2/c^2)}}, \quad E = \frac{mc^2}{\sqrt{1 - (v^2/c^2)}}.$$

The equations (B.21) are completely equivalent to equations (B.23) and (B.22). Note that equation (B.22) is a consequence of (B.23) just like the equation (B.21) with  $\mu = 0$  is also a consequence of the other three equations with spatial values for  $\mu$ .

The virtue of equations (B.21) is the *manifest covariance* of these equations, since linearly transforming equations between 4-vectors must hold in every inertial frame. Contrary to this, covariance is *not apparent* in the equations (B.22, B.23), but since they are equivalent to the manifestly covariant equations (B.21), they also must hold in every inertial frame. Covariance is only *hidden* in the nonlinear transformation behavior of equations (B.22, B.23). However, for practical purposes the equations (B.22, B.23) are often more useful.

The relativistic Lagrange function for a charged particle in terms of the laboratory time  $t$  is

$$L_{(t)} = -mc\sqrt{c^2 - \dot{\mathbf{x}}^2(t)} + q\dot{\mathbf{x}}(t) \cdot \mathbf{A}(\mathbf{x}(t), t) - q\Phi(\mathbf{x}(t), t). \quad (\text{B.24})$$

This yields the canonical momentum

$$\mathbf{p}_{can} = \frac{\partial L_{(t)}}{\partial \dot{\mathbf{x}}} = \frac{m\mathbf{c}\mathbf{v}}{\sqrt{c^2 - v^2}} + q\mathbf{A} = \mathbf{p} + q\mathbf{A},$$

and the equations of motion in the form (B.23). The relativistic action is

$$\begin{aligned} S &= \int dt L_{(t)} = \int \left( -mc\sqrt{c^2 dt^2 - d\mathbf{x}^2} + qd\mathbf{x} \cdot \mathbf{A} - qdt\Phi \right) \\ &= \int d\tau \left( -mc\sqrt{-\eta_{\mu\nu} \frac{dx^\mu}{d\tau} \frac{dx^\nu}{d\tau}} + qA_\mu \frac{dx^\mu}{d\tau} \right) = \int d\tau L_{(\tau)}. \end{aligned} \quad (\text{B.25})$$

The formulation in terms of the eigentime  $\tau$  of the particle yields the canonical momentum (use  $\eta_{\mu\nu} (dx^\mu/d\tau)(dx^\nu/d\tau) = -c^2$  from the equation  $c^2 d\tau^2 = -\eta_{\mu\nu} dx^\mu dx^\nu$  after the derivative)

$$p_{can,\mu} = \frac{\partial L_{(\tau)}}{\partial \dot{x}^\mu} = m\eta_{\mu\nu} \frac{dx^\nu}{d\tau} + qA_\mu = p_\mu + qA_\mu,$$

and the Lagrange equation is the manifestly covariant formulation (B.21) of the equations of motion.

The gauge-dependent contributions  $qA_\mu$  to the conserved momenta disappear in the fully covariant energy-momentum tensor of a classical charged particle of mass  $m$  and charge  $q$  coupled to electromagnetic fields,

$$\begin{aligned} T_\nu{}^\mu &= \frac{1}{\mu_0} \left( F_{\nu\rho} F^{\mu\rho} - \frac{1}{4} \eta_\nu{}^\mu F_{\rho\sigma} F^{\rho\sigma} \right) + \int d\tau mc U_\nu(\tau) U^\mu(\tau) \delta(x - x(\tau)) \\ &= \frac{1}{\mu_0} \left( F_{\nu\rho} F^{\mu\rho} - \frac{1}{4} \eta_\nu{}^\mu F_{\rho\sigma} F^{\rho\sigma} \right) + mc \frac{v_\nu v^\mu}{\sqrt{c^2 - v^2}} \delta(\mathbf{x} - \mathbf{x}(t)). \end{aligned} \quad (\text{B.26})$$

Contrary to the 4-velocity  $U^\mu$ , the four quantities  $v^\mu = dx^\mu/dt = U^\mu/\gamma = (c, \mathbf{v})$  are not components of a 4-vector, but still convenient for the representation of the classical energy-momentum tensor after integration over the eigentime of the particle.

The corresponding results for the energy density, energy current density and momentum density of the classical particle plus fields system are

$$\mathcal{H} = c\mathcal{P}^0 = T^{00} = \frac{\epsilon_0}{2} \mathbf{E}^2 + \frac{1}{2\mu_0} \mathbf{B}^2 + \frac{mc^3}{\sqrt{c^2 - v^2}} \delta(\mathbf{x} - \mathbf{x}(t)), \quad (\text{B.27})$$

$$\mathcal{S} = ce_i T^{0i} = \frac{1}{\mu_0} \mathbf{E} \times \mathbf{B} + \frac{mc^3 \mathbf{v}}{\sqrt{c^2 - v^2}} \delta(\mathbf{x} - \mathbf{x}(t)), \quad (\text{B.28})$$

$$\mathcal{P} = \frac{1}{c} \mathbf{e}_i T^{i0} = \epsilon_0 \mathbf{E} \times \mathbf{B} + \frac{mc\mathbf{v}}{\sqrt{c^2 - v^2}} \delta(\mathbf{x} - \mathbf{x}(t)) = \frac{1}{c^2} \mathcal{S}, \quad (\text{B.29})$$

and the stress tensor is

$$\begin{aligned} \underline{T} &= \left( \frac{\epsilon_0}{2} \mathbf{E}^2 + \frac{1}{2\mu_0} \mathbf{B}^2 \right) \underline{1} - \epsilon_0 \mathbf{E} \otimes \mathbf{E} - \frac{1}{\mu_0} \mathbf{B} \otimes \mathbf{B} \\ &\quad + mc \frac{\mathbf{v} \otimes \mathbf{v}}{\sqrt{c^2 - v^2}} \delta(\mathbf{x} - \mathbf{x}(t)). \end{aligned} \quad (\text{B.30})$$

## Relativistic center of mass frame

Considerations of two-particle systems in relativistic quantum mechanics also require the relativistic notion of center of mass frames. If two particles have momenta  $\mathbf{p}_1$  and  $\mathbf{p}_2$  in an inertial frame, every inertial frame with the property that the total momentum  $\mathbf{P}' = \mathbf{p}'_1 + \mathbf{p}'_2$  of the two-particle system in that frame vanishes is traditionally denoted as a center of mass frame for the two-particle system, although “zero total momentum frame” would be a more appropriate name. We will nevertheless continue to use the traditional name “center of mass frame”. Two center of mass frames for the system then differ at most by a combination of a translation and a rotation and possibly an inversion of the time axis. According

to equation (B.6) the task to actually transform into a center of mass frame then amounts to find a Lorentz boost into a frame moving with velocity  $\mathbf{v} = c\boldsymbol{\beta}$  such that with  $E = E_1 + E_2$

$$\mathbf{P}'_{\parallel} = \gamma\mathbf{P}_{\parallel} - \gamma\boldsymbol{\beta}\frac{E}{c} = 0 \tag{B.31}$$

and

$$\mathbf{P}'_{\perp} = \mathbf{P}_{\perp} = 0. \tag{B.32}$$

The condition (B.32) implies that we have to choose  $\boldsymbol{\beta} \parallel \mathbf{P}$ , and that  $\mathbf{P}_{\parallel} = \mathbf{P}, \mathbf{P}'_{\parallel} = \mathbf{P}'$ . The condition (B.31) is then solved by

$$\begin{aligned} \boldsymbol{\beta} &= c\frac{\mathbf{P}}{E}, \\ \gamma &= \frac{E}{\sqrt{E^2 - c^2\mathbf{P}^2}}. \end{aligned} \tag{B.33}$$

The momentum vectors of the two particles in the center of mass frame are therefore

$$\mathbf{p}'_{1,\perp} = \mathbf{p}_{1,\perp} = -\mathbf{p}_{2,\perp} = -\mathbf{p}'_{2,\perp},$$

and

$$\mathbf{p}'_{1,\parallel} = \frac{E}{\sqrt{E^2 - c^2\mathbf{P}^2}} \left( \mathbf{p}_{1,\parallel} - \frac{\mathbf{P}}{E}E_1 \right) = \frac{E_2\mathbf{p}_{1,\parallel} - E_1\mathbf{p}_{2,\parallel}}{\sqrt{E^2 - c^2\mathbf{P}^2}} = -\mathbf{p}'_{2,\parallel}.$$

The corresponding energies in the center of mass frame are

$$\begin{aligned} E'_1 &= \frac{E}{\sqrt{E^2 - c^2\mathbf{P}^2}} \left( E_1 - c^2\frac{\mathbf{P}}{E} \cdot \mathbf{p}_{1,\parallel} \right) = \frac{E_1^2 - c^2\mathbf{p}_1^2 + E_1E_2 - c^2\mathbf{p}_1 \cdot \mathbf{p}_2}{\sqrt{E^2 - c^2\mathbf{P}^2}}, \\ E'_2 &= \frac{E_2^2 - c^2\mathbf{p}_2^2 + E_1E_2 - c^2\mathbf{p}_1 \cdot \mathbf{p}_2}{\sqrt{E^2 - c^2\mathbf{P}^2}}. \end{aligned}$$

For consistency we notice

$$E' = E'_1 + E'_2 = \sqrt{E^2 - c^2\mathbf{P}^2},$$

as also implied by  $P'^2 = P^2$  with  $\mathbf{P}' = 0$ .

We also note that if we define the center of energy of the two-particle system,

$$\mathbf{R} = \frac{\mathbf{x}_1 E_1 + \mathbf{x}_2 E_2}{E_1 + E_2},$$

and if the particles do not interact, then the center of energy velocity is exactly the velocity (B.33) of the center of mass frame,

$$\dot{\mathbf{R}} = c^2 \frac{\mathbf{p}_1 + \mathbf{p}_2}{E_1 + E_2} = c\boldsymbol{\beta}.$$

If the particles interact, we need to also take into account the contributions from the fields which mediate the interactions to the center of energy and to the energy and momentum balances of the system, see (18.128, 18.129).

# Appendix C: Completeness of Sturm-Liouville Eigenfunctions

Completeness of eigenfunctions of self-adjoint operators is very important in quantum mechanics. Formulating exact theorems and proofs in general situations is a demanding mathematical problem. However, the setting of Sturm-Liouville problems with homogeneous boundary conditions in one dimension is sufficiently simple to be treated in a single appendix.

## Sturm-Liouville problems

Sturm-Liouville problems are linear boundary value problems consisting of a second order differential equation

$$\frac{d}{dx} \left( g(x) \frac{d\psi(x)}{dx} \right) - V(x)\psi(x) + E\varrho(x)\psi(x) = 0 \quad (\text{C.1})$$

in an interval  $a \leq x \leq b$  and homogeneous boundary conditions<sup>1</sup> (Sturm 1836, Liouville 1837)

$$\psi(a) = 0, \quad \psi(b) = 0. \quad (\text{C.2})$$

The functions  $g(x)$ ,  $V(x)$  and  $\varrho(x)$  are real and continuous in  $a \leq x \leq b$ , and we also assume that the functions  $g(x)$  and  $\varrho(x)$  are positive in  $a \leq x \leq b$ .

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<sup>1</sup>General Sturm-Liouville boundary conditions would only require linear combinations of  $\psi(x)$  and  $\psi'(x)$  to vanish at the boundaries, but for our purposes it is sufficient to impose the special conditions  $\psi(a) = 0$ ,  $\psi(b) = 0$ .

In ket notation without reference to a particular representation, we would write equation (C.1) as

$$E\varrho(x)|\psi(E)\rangle = \frac{1}{\hbar^2}p g(x)p|\psi(E)\rangle + V(x)|\psi(E)\rangle.$$

We can assume  $\psi(x) \equiv \langle x|\psi(E)\rangle$  to be a real function, and in this appendix we always assume that  $a$  and  $b$  are finite. We also require first order differentiability of  $g(x)$  and continuity of  $V(x)$  and  $\varrho(x)$ .

We can also assume  $\psi'(a) > 0$ . We know that  $\psi'(a) \neq 0$  because  $\psi'(a) = 0$  together with  $\psi(a) = 0$  and the Sturm-Liouville equation (C.1) would imply  $\psi(x) = 0$ . Furthermore, linearity of the Sturm-Liouville equation implies that we can always change the sign of  $\psi(x)$  to ensure  $\psi'(a) > 0$ .

Multiplication of equation (C.1) with  $\psi(x)$  and integration yields

$$H[\psi] \equiv \int_a^b dx (g(x)\psi'^2(x) + V(x)\psi^2(x)) = E \int_a^b dx \varrho(x)\psi^2(x) \equiv E\langle\psi|\psi\rangle$$

where the last equation defines the scalar product

$$\langle\phi|\psi\rangle = \int_a^b dx \varrho(x)\phi(x)\psi(x). \quad (\text{C.3})$$

It is easy to prove that (C.3) defines a scalar product since  $\langle\psi|\psi\rangle \geq 0$  and  $\langle\psi|\psi\rangle = 0 \Leftrightarrow \psi(x) = 0$ , and

$$0 \leq \langle\psi + \lambda\phi|\psi + \lambda\phi\rangle = \langle\psi|\psi\rangle + 2\lambda\langle\psi|\phi\rangle + \lambda^2\langle\phi|\phi\rangle \quad (\text{C.4})$$

has a minimum for

$$\lambda = -\frac{\langle\psi|\phi\rangle}{\langle\phi|\phi\rangle},$$

which after substitution in (C.4) yields the Schwarz inequality

$$\langle\psi|\phi\rangle^2 \leq \langle\psi|\psi\rangle\langle\phi|\phi\rangle.$$

The Sturm-Liouville equation (C.1) arises as an Euler-Lagrange equation from variation of the action

$$\begin{aligned} S[\psi] &= E\langle\psi|\psi\rangle - H[\psi] \\ &= \int_a^b dx (E\varrho(x)\psi^2(x) - g(x)\psi'^2(x) - V(x)\psi^2(x)) \end{aligned} \quad (\text{C.5})$$

with fixed endpoints  $\psi(a)$  and  $\psi(b)$ .

The stationary values of  $S[\psi]$  for arbitrary fixed endpoints  $\psi(a)$  and  $\psi(b)$  are

$$S[\psi] \Big|_{\text{on-shell}} = g(a)\psi(a)\psi'(a) - g(b)\psi(b)\psi'(b),$$

where the designation “on-shell” means that  $\psi(x)$  satisfies the Euler-Lagrange equation (C.1) of  $S[\psi]$ .

If we think of the Sturm-Liouville problem as a one-dimensional scalar field theory,  $G(x) = 1/4g^2(x)$  would play the role of a metric in  $a \leq x \leq b$  and  $H[\psi]$  would be the energy of the field  $\psi(x)$  if  $\psi(x)$  is normalized,  $\langle \psi | \psi \rangle = 1$ .

Suppose  $\psi_i(x)$  and  $\psi_j(x)$  are solutions of the Sturm-Liouville problem (C.1, C.2) with eigenvalues  $E_i$  and  $E_j$ , respectively. Use of the Sturm-Liouville equation (C.1) and partial integration yields

$$\begin{aligned} E_i \int_a^x d\xi \varrho(\xi) \psi_j(\xi) \psi_i(\xi) &= \int_a^x d\xi \psi_j(\xi) \left[ V(\xi) \psi_i(\xi) - \frac{d}{d\xi} \left( g(\xi) \frac{d}{d\xi} \psi_i(\xi) \right) \right] \\ &= \int_a^x d\xi \left( V(\xi) \psi_j(\xi) \psi_i(\xi) + g(\xi) \psi_j'(\xi) \psi_i'(\xi) \right) - g(x) \psi_j(x) \frac{d}{dx} \psi_i(x), \end{aligned}$$

and after another integration by parts we find

$$(E_i - E_j) \int_a^x d\xi \varrho(\xi) \psi_i(\xi) \psi_j(\xi) = g(x) \left( \psi_i(x) \frac{d}{dx} \psi_j(x) - \psi_j(x) \frac{d}{dx} \psi_i(x) \right). \quad (\text{C.6})$$

This equation implies for  $E_i = E_j$

$$\frac{d}{dx} \ln \psi_i(x) = \frac{d}{dx} \ln \psi_j(x),$$

i.e.  $\psi_i(x)$  has to be proportional to  $\psi_j(x)$ : There is no degeneracy of eigenvalues in the one-dimensional Sturm-Liouville problem.

For  $x = b$ , equation (C.6) implies the orthogonality property

$$(E_i - E_j) \langle \psi_i | \psi_j \rangle = 0$$

and taking into account the absence of degeneracy yields

$$\langle \psi_i | \psi_j \rangle \propto \delta_{ij}.$$

## Liouville’s normal form of Sturm’s equation

We can gauge the functions  $g(x)$  and  $\varrho(x)$  away through a transformation of variables

$$x \rightarrow X = \int_a^x d\xi \sqrt{\frac{\varrho(\xi)}{g(\xi)}}, \quad \psi(x) \rightarrow \Psi(X) = (\varrho(x)g(x))^{1/4} \psi(x).$$

This yields

$$0 \leq X \leq B = \int_a^b dx \sqrt{\frac{\varrho(x)}{g(x)}}, \quad \Psi(0) = 0, \quad \Psi(B) = 0,$$

and the Sturm-Liouville equation (C.1) assumes the form of a one-dimensional Schrödinger equation,

$$\frac{d^2}{dX^2} \Psi(X) - V(X)\Psi(X) + E\Psi(X) = 0 \quad (\text{C.7})$$

with

$$V(X) = \frac{V(x)}{\varrho(x)} + \frac{g(x)\varrho''(x) + \varrho(x)g''(x)}{4\varrho^2(x)} - \frac{5g(x)\varrho'^2(x)}{16\varrho^3(x)} - \frac{g'^2(x)}{16g(x)\varrho(x)} + \frac{g'(x)\varrho'(x)}{8\varrho^2(x)}.$$

Second order differentiability of  $\varrho(x)$  and  $g(x)$  is usually assumed. However, we only have to require continuity of the positive functions  $\varrho(x)$  and  $g(x)$  since we can deal with  $\delta$ -function singularities in one-dimensional potentials.

Equation (C.7) is *Liouville's normal form* of the Sturm-Liouville equation.

## Nodes of Sturm-Liouville eigenfunctions

For the following reasoning we assume that we have smoothly continued the functions  $V(x)$ ,  $\varrho(x) > 0$  and  $g(x) > 0$  for all values of  $x \in \mathbb{R}$ . It does not matter how we do that.

To learn more about the nodes of the eigenfunctions  $\psi_i(x)$  of the Sturm-Liouville boundary value problem, let us now assume that  $\psi(x, \lambda)$  and  $\psi(x, \mu)$  are solutions of the incomplete initial value problems

$$\lambda \varrho(x) \psi(x, \lambda) = V(x) \psi(x, \lambda) - \frac{d}{dx} \left( g(x) \frac{d\psi(x, \lambda)}{dx} \right), \quad \psi(a, \lambda) = 0, \quad (\text{C.8})$$

$$\mu \varrho(x) \psi(x, \mu) = V(x) \psi(x, \mu) - \frac{d}{dx} \left( g(x) \frac{d\psi(x, \mu)}{dx} \right), \quad \psi(a, \mu) = 0, \quad (\text{C.9})$$

with  $\lambda > \mu$ , but contrary to the boundary value problem (C.1, C.2) we do not impose any conditions at  $x = b$ . In that case there exist solutions to the Sturm-Liouville equations for arbitrary values of the parameters  $\lambda, \mu$ , and we can again require

$$\left. \frac{d\psi(x, \lambda)}{dx} \right|_{x=a} > 0, \quad \left. \frac{d\psi(x, \mu)}{dx} \right|_{x=a} > 0.$$

We recall the following facts from the theory of differential equations: The solution  $\psi(x, \lambda)$  to the initial value problem (C.8) is unique up to a multiplicative constant, and  $\psi(x, \lambda)$  depends continuously on the parameter  $\lambda$ .

The last fact is important, because it implies that the nodes  $y(\lambda)$  of  $\psi(x, \lambda)$ ,  $\psi(y(\lambda), \lambda) = 0$ , depend continuously on  $\lambda$ . Continuity of  $y(\lambda)$  is used in the demonstration below that the boundary value problem (C.1, C.2) has a solution for every value of  $b$ .

Multiplication of equation (C.8) with  $\psi(x, \mu)$  and equation (C.9) with  $\psi(x, \lambda)$ , integration from  $a$  to  $x > a$ , and subtraction of the equations yields

$$\begin{aligned} & (\lambda - \mu) \int_a^x d\xi \varrho(\xi) \psi(\xi, \lambda) \psi(\xi, \mu) \\ &= \int_a^x d\xi \left[ \psi(\xi, \lambda) \frac{d}{d\xi} \left( g(\xi) \frac{d\psi(\xi, \mu)}{d\xi} \right) - \psi(\xi, \mu) \frac{d}{d\xi} \left( g(\xi) \frac{d\psi(\xi, \lambda)}{d\xi} \right) \right] \\ &= g(x) \left( \psi(x, \lambda) \frac{d\psi(x, \mu)}{dx} - \psi(x, \mu) \frac{d\psi(x, \lambda)}{dx} \right). \end{aligned} \tag{C.10}$$

Now assume that  $y(\mu)$  is the first node of  $\psi(x, \mu)$  larger than  $a$ :

$$\psi(y(\mu), \mu) = 0, \quad y(\mu) > a.$$

Substituting  $x = y(\mu)$  in (C.10) yields

$$(\lambda - \mu) \int_a^{y(\mu)} dx \varrho(x) \psi(x, \lambda) \psi(x, \mu) = g(y(\mu)) \psi(y(\mu), \lambda) \left. \frac{d\psi(x, \mu)}{dx} \right|_{x=y(\mu)}. \tag{C.11}$$

We know that

$$(\lambda - \mu) \varrho(x) \psi(x, \mu) > 0$$

for  $a < x < y(\mu)$  and that

$$g(y(\mu)) \left. \frac{d\psi(x, \mu)}{dx} \right|_{x=y(\mu)} < 0.$$

This implies  $\psi(x, \lambda)$  must change its sign at least once for  $a < x < y(\mu)$ , and in particular  $y(\lambda) < y(\mu)$ :

*The location of the leftmost node  $y(\lambda) > a$  of the function  $\psi(x, \lambda)$  moves closer to  $a$  if  $\lambda$  increases.*

We are not really concerned with differentiability properties of the leftmost node  $y(\lambda)$ , but we can express the previous observation also as

$$y(\lambda) > a, \quad \frac{dy(\lambda)}{d\lambda} < 0.$$

Now assume that  $\lambda$  is small enough<sup>2</sup> so that even  $y(\lambda) > b$ . Then we can increase the parameter  $\lambda$  until we reach a value  $\lambda = E_1$  such that  $y(E_1) = b$ . This is then the lowest eigenvalue of our original Sturm-Liouville boundary value problem (C.1), and the corresponding eigenfunction is

$$\psi_1(x) = \psi(x, \lambda = E_1). \quad (\text{C.12})$$

*The eigenfunction  $\psi_1(x)$  for the lowest eigenvalue  $E_1$  has no nodes in  $a < x < b$ .*

Now we consider the first and the second node of  $\psi(x, \mu)$  for  $x > a$ ,

$$a < y(\mu) \equiv y_1(\mu) < y_2(\mu), \quad \psi(y_1(\mu), \mu) = 0, \quad \psi(y_2(\mu), \mu) = 0,$$

and we integrate from  $y_1(\mu)$  to  $y_2(\mu)$ ,

$$\begin{aligned} & (\lambda - \mu) \int_{y_1(\mu)}^{y_2(\mu)} dx \varrho(x) \psi(x, \lambda) \psi(x, \mu) \\ &= \int_{y_1(\mu)}^{y_2(\mu)} dx \left[ \psi(x, \lambda) \frac{d}{dx} \left( g(x) \frac{d\psi(x, \mu)}{dx} \right) - \psi(x, \mu) \frac{d}{dx} \left( g(x) \frac{d\psi(x, \lambda)}{dx} \right) \right] \\ &= g(y_2(\mu)) \psi(y_2(\mu), \lambda) \frac{d\psi(x, \mu)}{dx} \Big|_{x=y_2(\mu)} \\ &\quad - g(y_1(\mu)) \psi(y_1(\mu), \lambda) \frac{d\psi(x, \mu)}{dx} \Big|_{x=y_1(\mu)}. \end{aligned}$$

We know

$$(\lambda - \mu) \varrho(x) \psi(x, \mu) < 0$$

<sup>2</sup>The alert reader might worry that all  $y(\lambda)$  might be smaller than  $b$ , so that there is no finite small value  $\lambda$  with  $y(\lambda) > b$ , or otherwise that all  $y(\lambda)$  might be larger than  $b$ , so that no finite value  $E_1$  with  $y(E_1) = b$  would exist. These cases can be excluded through Sturm's comparison theorem, to be discussed later.

for  $y_1(\mu) < x < y_2(\mu)$ , and

$$g(y_1(\mu)) \frac{d\psi(x, \mu)}{dx} \Big|_{x=y_1(\mu)} < 0, \quad g(y_2(\mu)) \frac{d\psi(x, \mu)}{dx} \Big|_{x=y_2(\mu)} > 0.$$

This tells us that  $\psi(x, \lambda)$  has to change sign in the interval  $y_1(\mu) < x < y_2(\mu)$ , i.e. it must have at least one node there. We know that the first node  $y_1(\lambda) < y_1(\mu)$  is outside of this interval. Therefore we can infer that at least the second node  $y_2(\lambda)$  of  $\psi(x, \lambda)$  must be smaller than  $y_2(\mu)$ :  $y_2(\lambda) < y_2(\mu)$ . We can repeat this reasoning for the pair of adjacent nodes  $y_{n-1}(\mu), y_n(\mu)$  of  $\psi(x, \mu)$ , and we always find for  $\lambda > \mu$  that  $y_n(\lambda) < y_n(\mu)$ ,

$$a < y_n(\lambda), \quad \psi(y_n(\lambda), \lambda) = 0, \quad \frac{dy_n(\lambda)}{d\lambda} < 0.$$

*All nodes of the function  $\psi(x, \lambda)$  on the right hand side of  $x = a$  move closer to  $a$  if  $\lambda$  increases.*

Therefore we can repeat the reasoning above which had let us to the first solution  $\psi_1(x)$  with eigenvalue  $E_1$  of our Sturm-Liouville problem. To find the second eigenfunction, we increase  $\lambda > E_1$  until we hit a value  $\lambda = E_2$  such that  $y_2(E_2) = b$ , and the corresponding eigenfunction

$$\psi_2(x) = \psi(x, E_2)$$

will have exactly one node  $y_1(E_2)$  in the interval,  $a < y_1(E_2) < b$ .

The corresponding result for  $y_n(\lambda)$  tells us that in the  $n$ -th step we will find a parameter  $\lambda = E_n$  with  $y_n(E_n) = b$  and eigenfunction

$$\psi_n(x) = \psi(x, E_n),$$

and this function will have  $n - 1$  nodes  $a < y_1(E_n) < y_2(E_n) < \dots < y_{n-1}(E_n) < y_n(E_n) = b$  inside the interval.

### **Sturm's comparison theorem and estimates for the locations of the nodes $y_n(\lambda)$**

Sturm's comparison theorem makes a statement about the change of the nodes  $y_n > a$  of the solution  $\psi(x, \lambda)$  of

$$\frac{d}{dx} \left( g(x) \frac{d\psi(x, \lambda)}{dx} \right) + (\lambda q(x) - V(x)) \psi(x, \lambda) = 0, \quad \psi(a, \lambda) = 0, \quad (\text{C.13})$$

if the functions  $g(x)$ ,  $\varrho(x)$  and  $V(x)$  change. To prove the comparison theorem, we do *not* use Liouville's normal form, but perform the following simple transformation of variables,

$$X = \int_a^x \frac{dx'}{g(x')}, \quad \Psi(X, \lambda) = \psi(x, \lambda).$$

This transforms (C.13) into the following form,

$$\frac{d^2 \Psi(X, \lambda)}{dX^2} + (\lambda R(X) - V(X)) \Psi(X, \lambda) = 0, \quad \Psi(0, \lambda) = 0, \quad (\text{C.14})$$

$$R(X) = g(x)\varrho(x) > 0, \quad V(X) = g(x)V(x),$$

and the nodes  $Y_n > 0$  of  $\Psi(X, \lambda)$  are related to the nodes  $y_n > a$  of  $\psi(x, \lambda)$  through

$$Y_n = \int_a^{y_n} \frac{dx}{g(x)}. \quad (\text{C.15})$$

Now we consider another Sturm-Liouville problem of the form (C.14), but with different functions

$$\lambda S(X) - W(X) > \lambda R(X) - V(X),$$

$$\frac{d^2 \Phi(X, \lambda)}{dX^2} + (\lambda S(X) - W(X)) \Phi(X, \lambda) = 0, \quad \Phi(0, \lambda) = 0, \quad (\text{C.16})$$

and we denote the positive nodes of  $\Phi(X, \lambda)$  with  $Z_n$ . We also require again  $\Psi'(0) > 0$ ,  $\Phi'(0) > 0$ . Equations (C.14, C.16) imply

$$\begin{aligned} & \int_{Y_{n-1}}^{Y_n} dX [V(X) - W(X) - \lambda (R(X) - S(X))] \Psi(X, \lambda) \Phi(X, \lambda) \\ &= \Phi(Y_n, \lambda) \left. \frac{d\Psi(X, \lambda)}{dX} \right|_{X=Y_n} - \Phi(Y_{n-1}, \lambda) \left. \frac{d\Psi(X, \lambda)}{dX} \right|_{X=Y_{n-1}}. \end{aligned} \quad (\text{C.17})$$

The following terms in (C.17) have all the same sign,

$$\begin{aligned} & [V(X) - W(X) - \lambda (R(X) - S(X))] \Psi(X, \lambda) \Big|_{Y_{n-1} < X < Y_n}, \\ & \frac{d\Psi(X, \lambda)}{dX} \Big|_{X=Y_{n-1}}, \quad - \frac{d\Psi(X, \lambda)}{dX} \Big|_{X=Y_n}. \end{aligned}$$

This implies that  $\Phi(X, \lambda)$  must change its sign in  $Y_{n-1} < X < Y_n$ , and since this must hold for every  $n \geq 1$  we find

$$Z_n < Y_n.$$

Increasing  $\lambda R(X) - V(X)$  moves the nodes  $Y_n > 0$  of the function  $\Psi(X, \lambda)$  to the left. From this we can first derive bounds for the nodes  $Y_n > 0$  which arise from the nodes of the solutions of

$$\begin{aligned} &\Psi''_{min}(X, \lambda) + (\lambda R_{max} - V_{min}) \Psi_{min}(X, \lambda) \\ &= \Psi''_{min}(X, \lambda) + g_{max} (\lambda \varrho_{max} - U_{min}) \Psi_{min}(X, \lambda) = 0, \quad (C.18) \\ &\Psi_{min}(0, \lambda) = 0, \end{aligned}$$

and

$$\begin{aligned} &\Psi''_{max}(X, \lambda) + (\lambda R_{min} - V_{max}) \Psi_{max}(X, \lambda) \\ &= \Psi''_{max}(X, \lambda) + g_{min} (\lambda \varrho_{min} - U_{max}) \Psi_{max}(X, \lambda) = 0, \quad (C.19) \\ &\Psi_{max}(0, \lambda) = 0. \end{aligned}$$

Here we use the bounds of the continuous functions  $g(x)$ ,  $V(x)$ ,  $\varrho(x)$  on  $a \leq x \leq b$ ,

$$\begin{aligned} 0 < g_{min} \leq g(x) \leq g_{max}, \quad U_{min} \leq V(x) \leq U_{max}, \\ 0 < \varrho_{min} \leq \varrho(x) \leq \varrho_{max}. \end{aligned}$$

The solutions of both equations (C.18) and (C.19) have nodes if (recall that both  $g(x) > 0$  and  $\varrho(x) > 0$ )

$$\lambda > U_{min}/\varrho_{max},$$

and the two solutions are

$$\begin{aligned} \Psi_{min}(X, \lambda) &\propto \sin\left(\sqrt{g_{max} (\lambda \varrho_{max} - U_{min})} X\right), \\ \Psi_{max}(X, \lambda) &\propto \sin\left(\sqrt{g_{min} (\lambda \varrho_{min} - U_{max})} X\right). \end{aligned}$$

This yields bounds for the nodes  $Y_n > 0$  of  $\Psi(X, \lambda)$ ,

$$\frac{n\pi}{\sqrt{g_{max} (\lambda \varrho_{max} - U_{min})}} \leq Y_n \leq \frac{n\pi}{\sqrt{g_{min} (\lambda \varrho_{min} - U_{max})}}. \quad (C.20)$$

However, we also know from equation (C.15) that  $g_{min} Y_n \leq y_n - a \leq g_{max} Y_n$ , and therefore<sup>3</sup>

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<sup>3</sup>These bounds can be strengthened by a longer proof, but the present result is completely sufficient for our purposes.

$$a + \frac{g_{\min} n \pi}{\sqrt{g_{\max} (\lambda Q_{\max} - U_{\min})}} \leq y_n \leq a + \frac{g_{\max} n \pi}{\sqrt{g_{\min} (\lambda Q_{\min} - U_{\max})}}. \quad (\text{C.21})$$

This implies in particular that *there is no accumulation point for the nodes  $y_n$  of  $\psi(x, \lambda)$ , and  $y_n$  must grow like  $n$  for large  $n$ .*

For our previous proof that  $\psi_1(x)$  (C.12) has its first node at  $y_1 = b$ , we needed the assumption that there are small enough values of  $\lambda$  such that the first node  $y_1(\lambda)$  of  $\psi(x, \lambda)$  satisfies  $y_1(\lambda) > b$ . We can now confirm that from the lower bound in (C.21). It will suffice to choose

$$\frac{U_{\min}}{Q_{\max}} < \lambda < \frac{U_{\min}}{Q_{\max}} + \frac{g_{\min}^2 \pi^2}{Q_{\max} g_{\max} (b-a)^2}. \quad (\text{C.22})$$

We also needed the assumption that for large enough  $\lambda$  the first node  $y_1(\lambda) > a$  would be smaller than  $b$ . This is easily confirmed from the upper bound in (C.21). It is sufficient to choose

$$\lambda > \frac{U_{\max}}{Q_{\min}} + \frac{g_{\max}^2 \pi^2}{Q_{\min} g_{\min} (b-a)^2}. \quad (\text{C.23})$$

## Eigenvalue estimates for the Sturm-Liouville problem

We have found that the Sturm-Liouville boundary value problem (C.1, C.2) has an increasing, non-degenerate set of eigenvalues

$$E_1 < E_2 < \dots$$

and arises as an Euler-Lagrange equation for the action

$$\begin{aligned} S[\psi] &= E \langle \psi | \psi \rangle - H[\psi] \\ &= \int_a^b dx (E Q(x) \psi^2(x) - g(x) \psi'^2(x) - V(x) \psi^2(x)). \end{aligned} \quad (\text{C.24})$$

For every continuous function  $\psi(x)$  in  $a \leq x \leq b$  we define the normalized function

$$\hat{\psi}(x) = \frac{\psi(x)}{\sqrt{\langle \psi | \psi \rangle}}.$$

Since  $S[\psi]$  is homogeneous in  $\psi$ ,  $\psi(x)$  is a stationary point of  $S[\psi]$  if and only if  $\hat{\psi}(x)$  is a stationary point of

$$S[\hat{\psi}] = E - H[\hat{\psi}],$$

which implies also that  $\hat{\psi}(x)$  is a stationary point of the functional

$$H[\hat{\psi}] = \frac{H[\psi]}{\langle \psi | \psi \rangle} = \frac{\int_a^b dx [g(x)\psi'^2(x) + V(x)\psi^2(x)]}{\int_a^b dx \varrho(x)\psi^2(x)}. \tag{C.25}$$

We have already found that there is a discrete subset  $\hat{\psi}_n(x)$ ,  $n \in \mathbb{N}$ , of stationary points of  $H[\hat{\psi}]$  which satisfy the boundary conditions  $\hat{\psi}_n(a) = 0$ ,  $\hat{\psi}_n(b) = 0$ , and are mutually orthogonal,

$$\langle \hat{\psi}_m | \hat{\psi}_n \rangle = \delta_{mn}.$$

Use of the Sturm-Liouville equation and the boundary conditions yields the values of the functional  $H[\hat{\psi}]$  at the stationary points  $\hat{\psi}_n(x)$ ,

$$H[\hat{\psi}_n] = E_n.$$

We already know  $E_1 < E_2 < \dots$ , and therefore we have found that the functional  $H[\hat{\psi}]$  has a minimum

$$H[\hat{\psi}_1] = E_1$$

on the space of functions

$$\mathcal{F}_{a,b} = \{\psi(x), a \leq x \leq b | \psi(a) = 0, \psi(b) = 0, \langle \psi | \psi \rangle = 1\},$$

and in general we have a minimum

$$H[\hat{\psi}_n] = E_n$$

on the space of functions

$$\mathcal{F}_{a,b}^{(n)} = \{\psi(x), a \leq x \leq b | \psi(a) = 0, \psi(b) = 0, \langle \psi | \psi \rangle = 1, \langle \psi_i | \psi \rangle = 0, 1 \leq i \leq n-1\}.$$

The explicit form of  $H[\hat{\psi}]$  in equation (C.25) shows that all the eigenvalues  $E_n$  increase if  $g(x)$  increases or  $V(x)$  increases or  $\varrho(x)$  decreases.

However, those continuous functions must be bounded on the finite interval  $a \leq x \leq b$ ,

$$0 < g_{min} \leq g(x) \leq g_{max}, \quad U_{min} \leq V(x) \leq U_{max}, \\ 0 < \varrho_{min} \leq \varrho(x) \leq \varrho_{max}.$$

Therefore we can replace those functions with their extremal values to derive estimates for the eigenvalues  $E_n$ .

The Sturm-Liouville problems for the extremal values are

$$g_{\min/\max} \psi_n''(x) + (E_{n,\min/\max} Q_{\max/\min} - U_{\min/\max}) \psi_n(x) = 0,$$

$$\psi_n(a) = 0, \quad \psi_n(b) = 0,$$

with solutions

$$\psi_n(x) \propto \sin\left(n\pi \frac{x-a}{b-a}\right)$$

and corresponding eigenvalues

$$E_{n,\min/\max} = \frac{1}{Q_{\max/\min}} \left( U_{\min/\max} + g_{\min/\max} \frac{n^2 \pi^2}{(b-a)^2} \right).$$

This implies the bounds

$$\frac{1}{Q_{\max}} \left( U_{\min} + g_{\min} \frac{n^2 \pi^2}{(b-a)^2} \right) \leq E_n \leq \frac{1}{Q_{\min}} \left( U_{\max} + g_{\max} \frac{n^2 \pi^2}{(b-a)^2} \right). \quad (\text{C.26})$$

In particular, *at most a finite number of the lowest eigenvalues  $E_n$  can be negative, and the eigenvalues for large  $n$  must grow like  $n^2$ .*

Both of these observations are crucial for the proof that the set  $\psi_n(x)$  of eigenfunctions of the Sturm-Liouville problem (C.1, C.2) provide a complete basis for the expansion of piecewise continuous functions in  $a \leq x \leq b$ .

## Completeness of Sturm-Liouville eigenstates

We now assume that the Sturm-Liouville eigenstates are normalized,

$$\langle \psi_i | \psi_j \rangle = \delta_{ij}.$$

Let  $\phi(x)$  be an arbitrary smooth function on  $a \leq x \leq b$  with  $\phi(a) = 0$  and  $\phi(b) = 0$ , and define

$$\varphi_n(x) = \phi(x) - \sum_{i=1}^n \psi_i(x) \langle \psi_i | \phi \rangle.$$

Then we have

$$0 \leq \langle \varphi_n | \varphi_n \rangle = \langle \phi | \phi \rangle - \sum_{i=1}^n \langle \psi_i | \phi \rangle^2,$$

i.e. for all  $n$  we have a *Bessel inequality*

$$\langle \phi | \phi \rangle \geq \sum_{i=1}^n \langle \psi_i | \phi \rangle^2.$$

We also have  $\langle \varphi_n | \psi_i \rangle = 0$ ,  $1 \leq i \leq n$ , and  $\varphi_n(a) = 0$ ,  $\varphi_n(b) = 0$ , i.e.

$$\varphi_n(x) \in \mathcal{F}_{a,b}^{(n+1)}.$$

Therefore the minimum property of the eigenvalue  $E_{n+1}$  implies

$$E_{n+1} \leq \frac{H[\varphi_n]}{\langle \varphi_n | \varphi_n \rangle}. \quad (\text{C.27})$$

We have

$$\begin{aligned} H[\varphi_n] &= H[\phi] - 2 \sum_{i=1}^n \langle \psi_i | \phi \rangle \int_a^b dx (g(x)\phi'(x)\psi_i'(x) + V(x)\phi(x)\psi_i(x)) \\ &\quad + \sum_{i,j=1}^n \langle \psi_i | \phi \rangle \langle \psi_j | \phi \rangle \int_a^b dx (g(x)\psi_i'(x)\psi_j'(x) + V(x)\psi_i\psi_j(x)). \end{aligned}$$

In the first sum, partial integration and use of the Sturm-Liouville equation yields

$$\begin{aligned} \int_a^b dx (g(x)\phi'(x)\psi_i'(x) + V(x)\phi(x)\psi_i(x)) &= E_i \int_a^b dx \varrho(x)\phi(x)\psi_i(x) \\ &= E_i \langle \psi_i | \phi \rangle. \end{aligned}$$

In the double sum, partial integration and use of the Sturm-Liouville equation yields

$$\begin{aligned} \int_a^b dx (g(x)\psi_i'(x)\psi_j'(x) + V(x)\psi_i\psi_j(x)) &= E_i \int_a^b dx \varrho(x)\psi_i(x)\psi_j(x) \\ &= E_i \delta_{ij}. \end{aligned}$$

This implies

$$H[\varphi_n] = H[\phi] - \sum_{i=1}^n E_i \langle \psi_i | \phi \rangle^2. \quad (\text{C.28})$$

Since at most finitely many of the eigenvalues  $E_i$  can be negative, equation (C.28) tells us that the functional  $H[\varphi_n]$  must remain bounded from above for  $n \rightarrow \infty$ , e.g. for

$$E_1 < E_2 < \dots < E_N < 0 \leq E_{N+1} < \dots$$

we have the bound

$$H[\varphi_n] \leq H[\phi] + \sum_{i=1}^N |E_i| \langle \psi_i | \phi \rangle^2.$$

On the other hand, equation (C.27) yields for  $n > N$  (to ensure  $E_{n+1} > 0$ ),

$$\langle \varphi_n | \varphi_n \rangle = \langle \phi | \phi \rangle - \sum_{i=1}^n \langle \psi_i | \phi \rangle^2 \leq \frac{H[\varphi_n]}{E_{n+1}}$$

and since  $E_{n+1}$  grows like  $n^2$  for large  $n$  while  $H[\varphi_n]$  must remain bounded, we find the completeness relation

$$\lim_{n \rightarrow \infty} \langle \varphi_n | \varphi_n \rangle = \lim_{n \rightarrow \infty} \int_a^b dx \varrho(x) \left( \phi(x) - \sum_{i=1}^n \psi_i(x) \langle \psi_i | \phi \rangle \right)^2 = 0 \quad (\text{C.29})$$

or equivalently,

$$\langle \phi | \phi \rangle = \lim_{n \rightarrow \infty} \sum_{i=1}^n \langle \phi | \psi_i \rangle \langle \psi_i | \phi \rangle.$$

Completeness of the series

$$\sum_{i=1}^{\infty} \psi_i(x) \langle \psi_i | \phi \rangle \sim \phi(x)$$

in the sense of equation (C.29) is denoted as *completeness in the mean*, and is sometimes also expressed as

$$\text{l.i.m.}_{n \rightarrow \infty} \sum_{i=1}^n \psi_i(x) \langle \psi_i | \phi \rangle = \phi(x),$$

where l.i.m. stands for “limit in the mean”. Completeness in the mean says that the series  $\sum_{i=1}^{\infty} \psi_i(x) \langle \psi_i | \phi \rangle$  approximates  $\phi(x)$  in the least squares sense.

Completeness in the mean also implies for the two piecewise continuous functions  $f$  and  $g$

$$f(x) \pm g(x) \sim \sum_{i=1}^{\infty} \psi_i(x) \langle \psi_i | f \rangle \pm \sum_{i=1}^{\infty} \psi_i(x) \langle \psi_i | g \rangle$$

and therefore

$$\langle f | g \rangle = \frac{1}{4} (\langle f + g | f + g \rangle - \langle f - g | f - g \rangle) = \lim_{n \rightarrow \infty} \sum_{i=1}^n \langle f | \psi_i \rangle \langle \psi_i | g \rangle. \quad (\text{C.30})$$

Completeness in the sense of (C.30) is enough for quantum mechanics, because it says that we can use the completeness relation

$$\mathbb{1} = \lim_{n \rightarrow \infty} \sum_{i=1}^n |\psi_i\rangle\langle\psi_i|$$

in the calculation of matrix elements between sufficiently smooth functions (where “sufficiently smooth = continuously differentiable to a required order” depends on the operators we use). This is all that is really needed in quantum mechanics. However, for piecewise smooth functions, the relation also holds pointwise almost everywhere (see Remark 3 below).

I would like to add a few remarks:

1. The completeness property (C.29) also applies to piecewise continuous functions in  $a \leq x \leq b$  and functions which do not vanish at the boundary points, because every piecewise continuous function can be approximated in the mean by a smooth function which vanishes at the boundaries.
2. If  $\phi(x)$  is a smooth function satisfying the Sturm-Liouville boundary conditions, as we have assumed in the derivation of (C.29), the series under the integral sign will even converge uniformly to  $\phi(x)$ ,

$$\lim_{n \rightarrow \infty} \sum_{i=1}^n \psi_i(x)\langle\psi_i|\phi\rangle = \phi(x),$$

i.e. for all  $a \leq x \leq b$  and all values  $\epsilon > 0$ , there exists an  $n(\epsilon)$  such that

$$\left| \phi(x) - \sum_{i=1}^n \psi_i(x)\langle\psi_i|\phi\rangle \right| < \epsilon \quad \text{if } n \geq n(\epsilon). \tag{C.31}$$

Uniformity of the convergence refers to the fact that the same  $n(\epsilon)$  ensures (C.31) for all  $a \leq x \leq b$ .

3. If  $\phi(x)$  is piecewise smooth in  $a \leq x \leq b$ , it can still be expanded pointwise in Sturm-Liouville eigenstates. Except for points of discontinuity of  $\phi(x)$ , and except for the boundary points if  $\phi(x)$  does not satisfy the same boundary conditions as the eigenfunctions  $\psi_i(x)$ , the expansion

$$\phi(x) = \lim_{n \rightarrow \infty} \sum_{i=1}^n \psi_i(x)\langle\psi_i|\phi\rangle$$

holds pointwise, and the series converges uniformly to  $\phi(x)$  in every closed interval which excludes discontinuities of  $\phi(x)$  (and the series converges to the arithmetic mean in the points of discontinuity). The boundary points must also be excluded if  $\phi(x)$  does not satisfy the Sturm-Liouville boundary conditions.

## Appendix D: Properties of Hermite Polynomials

We use the following equation as a definition of Hermite polynomials,

$$H_n(x) = \exp\left(\frac{1}{2}x^2\right) \left(x - \frac{d}{dx}\right)^n \exp\left(-\frac{1}{2}x^2\right), \quad (\text{D.1})$$

because we initially encountered them in this form in the solution of the harmonic oscillator in Chapter 6. We can use the identity

$$\left(x + \frac{d}{dx}\right)f(x) = \exp\left(-\frac{1}{2}x^2\right) \frac{d}{dx} \left[\exp\left(\frac{1}{2}x^2\right)f(x)\right]$$

to rewrite equation (D.1) in the form

$$\begin{aligned} H_n(x) &= \exp\left(\frac{1}{2}x^2\right) \left[2x - \exp\left(-\frac{1}{2}x^2\right) \frac{d}{dx} \exp\left(\frac{1}{2}x^2\right)\right]^n \exp\left(-\frac{1}{2}x^2\right) \\ &= \left[\exp\left(\frac{1}{2}x^2\right) \left[2x - \exp\left(-\frac{1}{2}x^2\right) \frac{d}{dx} \exp\left(\frac{1}{2}x^2\right)\right] \exp\left(-\frac{1}{2}x^2\right)\right]^n \\ &= \left(2x - \frac{d}{dx}\right)^n 1, \end{aligned} \quad (\text{D.2})$$

or we can use the identity

$$\left(x - \frac{d}{dx}\right)f(x) = -\exp\left(\frac{1}{2}x^2\right) \frac{d}{dx} \left[\exp\left(-\frac{1}{2}x^2\right)f(x)\right]$$

to rewrite equation (D.1) in the Rodrigues form

$$H_n(x) = \exp(x^2) \left(-\frac{d}{dx}\right)^n \exp(-x^2). \quad (\text{D.3})$$

The Rodrigues formula implies

$$\begin{aligned} \sum_{n=0}^{\infty} H_n(x) \frac{z^n}{n!} &= \sum_{n=0}^{\infty} \left[ \exp(x^2) \frac{\partial^n}{\partial z^n} \exp(-(x-z)^2) \right]_{z=0} \frac{z^n}{n!} \\ &= \exp(x^2) \exp(-(x-z)^2) = \exp(2xz - z^2). \end{aligned} \quad (\text{D.4})$$

The residue theorem then also yields the representation

$$H_n(x) = \frac{n!}{2\pi i} \oint dz \frac{\exp(2xz - z^2)}{z^{n+1}}, \quad (\text{D.5})$$

where the integration contour encloses  $z = 0$  in the positive sense of direction, i.e. counter clockwise.

Another useful integral representation for the Hermite polynomials follows from (D.2) and the equation

$$\begin{aligned} \int_{-\infty}^{\infty} du (2u)^n \exp(-(u+v)^2) &= \int_{-\infty}^{\infty} du \left( -2v - \frac{\partial}{\partial v} \right)^n \exp(-(u+v)^2) \\ &= \left( -2v - \frac{\partial}{\partial v} \right)^n \sqrt{\pi}. \end{aligned}$$

This yields in particular for  $v = -ix$ ,

$$\int_{-\infty}^{\infty} du (2u)^n \exp(-(u-ix)^2) = i^n \sqrt{\pi} H_n(x). \quad (\text{D.6})$$

Combination of equations (D.4) and (D.6) yields Mehler's formula<sup>1</sup>,

$$\begin{aligned} \sum_{n=0}^{\infty} H_n(x) H_n(x') \frac{z^n}{n!} &= \sum_{n=0}^{\infty} H_n(x) \frac{1}{\sqrt{\pi} n!} \int_{-\infty}^{\infty} du (-2iuz)^n \exp(-(u-ix')^2) \\ &= \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} du \exp(-4ixuz + 4u^2 z^2) \exp(-(u-ix')^2) \\ &= \frac{1}{\sqrt{1-4z^2}} \exp\left(-4z \frac{z(x^2 + x'^2) - xx'}{1-4z^2}\right). \end{aligned} \quad (\text{D.7})$$

This requires  $|z| < 1/2$  for convergence. In Sections 6.3 and 13.1 we need this in the form for  $|z| < 1$ ,

<sup>1</sup>F.G. Mehler, J. Math. 66, 161 (1866).

$$\begin{aligned}
& \sum_{n=0}^{\infty} H_n(x)H_n(x') \frac{z^n}{2^n n!} \exp\left(-\frac{x^2 + x'^2}{2}\right) \\
&= \frac{1}{\sqrt{1-z^2}} \exp\left(-\frac{(1+z^2)(x^2 + x'^2) - 4zx x'}{2(1-z^2)}\right). \tag{D.8}
\end{aligned}$$

Indeed, applications of this equation for the harmonic oscillator are usually in the framework of distributions and require the limit  $|z| \rightarrow 1$ . In principle we should therefore replace the corresponding phase factors  $z$  in Sections 6.3 and 13.1 with  $z \exp(-\epsilon)$ , and take the limit  $\epsilon \rightarrow +0$  after applying any distributions which are derived from (D.8).

# Appendix E: The Baker-Campbell-Hausdorff Formula

The Baker-Campbell-Hausdorff formula explains how to combine the product of operator exponentials  $\exp(A) \cdot \exp(B)$  into a single operator exponential  $\exp[\Phi(A, B)]$ , if the series expansion for  $\Phi(A, B)$  provided by the Baker-Campbell-Hausdorff formula converges.

We try to determine  $\Phi(A, B)$  as a power series in a parameter  $\lambda$ ,

$$\exp[\lambda A] \cdot \exp[\lambda B] = \exp[\Phi(\lambda A, \lambda B)], \quad \Phi(\lambda A, \lambda B) = \sum_{n=1}^{\infty} \lambda^n c_n(A, B).$$

We also use the notation of the adjoint action of an operator  $A$  on an operator  $B$ ,

$$A^{(ad)} \circ B = -[A, B].$$

We start with

$$\exp[\alpha A] \cdot \exp[\beta B] = \exp[\Phi(\alpha A, \beta B)].$$

This implies with Lemma (6.22) the equations

$$\begin{aligned} B &= \exp[-\Phi(\alpha A, \beta B)] \frac{\partial}{\partial \beta} \exp[\Phi(\alpha A, \beta B)] = \sum_{n=1}^{\infty} \frac{(-)^n}{n!} [\Phi(\alpha A, \beta B), \partial_\beta] \\ &= - \sum_{n=1}^{\infty} \frac{(-)^n}{n!} [ \Phi(\alpha A, \beta B), \partial_\beta \Phi(\alpha A, \beta B) ] \\ &= \sum_{n=1}^{\infty} \frac{1}{n!} (\Phi(\alpha A, \beta B)^{(ad)})^{n-1} \circ \partial_\beta \Phi(\alpha A, \beta B) \\ &= \frac{\exp[\Phi(\alpha A, \beta B)^{(ad)}] - 1}{\Phi(\alpha A, \beta B)^{(ad)}} \circ \partial_\beta \Phi(\alpha A, \beta B) \end{aligned}$$

and

$$\begin{aligned}
 A &= -\exp[\Phi(\alpha A, \beta B)] \frac{\partial}{\partial \alpha} \exp[-\Phi(\alpha A, \beta B)] = -\sum_{n=1}^{\infty} \frac{1}{n!} {}^n [\Phi(\alpha A, \beta B), \partial_\alpha] \\
 &= \sum_{n=1}^{\infty} \frac{1}{n!} {}^{n-1} [\Phi(\alpha A, \beta B), \partial_\alpha \Phi(\alpha A, \beta B)] \\
 &= \sum_{n=1}^{\infty} \frac{1}{n!} (-\Phi(\alpha A, \beta B)^{(ad)})^{n-1} \circ \partial_\alpha \Phi(\alpha A, \beta B) \\
 &= \frac{1 - \exp[-\Phi(\alpha A, \beta B)^{(ad)}]}{\Phi(\alpha A, \beta B)^{(ad)}} \circ \partial_\alpha \Phi(\alpha A, \beta B).
 \end{aligned}$$

For the inversion of these equations, we notice

$$\begin{aligned}
 \left( \frac{\exp(z) - 1}{z} \right)^{-1} &= \frac{z}{\exp(z) - 1} = z \frac{\exp(-z/2)}{\exp(z/2) - \exp(-z/2)} \\
 &= \frac{z}{2} \frac{\exp(z/2) + \exp(-z/2)}{\exp(z/2) - \exp(-z/2)} - \frac{z}{2} \\
 &= \frac{z}{2} \coth \frac{z}{2} - \frac{z}{2} = 1 + \sum_{n=1}^{\infty} \frac{(-)^{n+1}}{(2n)!} B_n z^{2n} - \frac{z}{2}, \\
 \left( \frac{1 - \exp(-z)}{z} \right)^{-1} &= \frac{z}{1 - \exp(-z)} = z \frac{\exp(z/2)}{\exp(z/2) - \exp(-z/2)} \\
 &= \frac{z}{2} \frac{\exp(z/2) + \exp(-z/2)}{\exp(z/2) - \exp(-z/2)} + \frac{z}{2} \\
 &= \frac{z}{2} \coth \frac{z}{2} + \frac{z}{2} = 1 + \sum_{n=1}^{\infty} \frac{(-)^{n+1}}{(2n)!} B_n z^{2n} + \frac{z}{2},
 \end{aligned}$$

where the coefficients  $B_n$  are Bernoulli numbers.

The previous equations yield (with  $\Phi(\alpha A, \beta B)^{(ad)} \circ A = -[\Phi(\alpha A, \beta B), A]$ )

$$\begin{aligned}
 \partial_\alpha \Phi(\alpha A, \beta B) &= \frac{\Phi(\alpha A, \beta B)^{(ad)}}{2} \coth \frac{\Phi(\alpha A, \beta B)^{(ad)}}{2} \circ A \\
 &\quad - \frac{1}{2} [\Phi(\alpha A, \beta B), A], \\
 \partial_\beta \Phi(\alpha A, \beta B) &= \frac{\Phi(\alpha A, \beta B)^{(ad)}}{2} \coth \frac{\Phi(\alpha A, \beta B)^{(ad)}}{2} \circ B \\
 &\quad + \frac{1}{2} [\Phi(\alpha A, \beta B), B],
 \end{aligned}$$

$$\begin{aligned} \partial_\lambda \Phi(\lambda A, \lambda B) &= \left[ \partial_\alpha \Phi(\alpha A, \beta B) + \partial_\beta \Phi(\alpha A, \beta B) \right]_{\alpha=\beta=\lambda} \\ &= \frac{\Phi(\lambda A, \lambda B)^{(ad)}}{2} \coth \frac{\Phi(\lambda A, \lambda B)^{(ad)}}{2} \circ (A + B) \\ &\quad + \frac{1}{2} [A - B, \Phi(\lambda A, \lambda B)], \end{aligned}$$

i.e.

$$\begin{aligned} \partial_\lambda \Phi(\lambda A, \lambda B) &= A + B + \sum_{n=1}^{\infty} \frac{(-)^{n+1}}{(2n)!} B_n \cdot [\Phi(\lambda A, \lambda B)^{(ad)]^{2n} \circ (A + B) \\ &\quad + \frac{1}{2} [A - B, \Phi(\lambda A, \lambda B)]. \end{aligned} \tag{E.1}$$

Equation (E.1) provides us with a recursion relation for the  $n$ -th order coefficient functions  $c_n(A, B)$ ,

$$\begin{aligned} (n + 1)c_{n+1}(A, B) &= \frac{1}{2} [A - B, c_n(A, B)] + \sum_{m=1}^{\lfloor n/2 \rfloor} \frac{(-)^{m+1}}{(2m)!} B_m \\ &\times \sum_{\substack{1 \leq k_1, k_2, \dots, k_{2m} \\ k_1 + \dots + k_{2m} = n}} [c_{k_{2m}}(A, B), [\dots, [c_{k_2}(A, B), [c_{k_1}(A, B), A + B]] \dots]], \end{aligned} \tag{E.2}$$

with

$$c_0(A, B) = 0, \quad c_1(A, B) = A + B.$$

The floor function  $\lfloor x \rfloor$  maps to the next lowest integer smaller or equal to  $x$ , i.e.  $\lfloor n/2 \rfloor = n/2$  if  $n$  is even,  $\lfloor n/2 \rfloor = (n - 1)/2$  if  $n$  is odd.

The result (E.2) yields for the next three terms

$$\begin{aligned} c_2(A, B) &= \frac{1}{2} [A, B], \\ c_3(A, B) &= \frac{1}{12} [A - B, [A, B]] + \frac{1}{6} B_1 [A + B, [A + B, A + B]] \\ &= \frac{1}{12} [A, [A, B]] + \frac{1}{12} [B, [B, A]], \\ c_4(A, B) &= \frac{1}{96} [A - B, [A, [A, B]] + [B, [B, A]]] \\ &\quad + \frac{1}{16} B_1 [A + B, [[A, B], A + B]] \end{aligned}$$

$$\begin{aligned}
&= \frac{1}{96} \left( [A, [A, [A, B]]] - [B, [B, [B, A]]] + [A, [B, [B, A]]] \right. \\
&\quad - [B, [A, [A, B]]] - [A, [A, [A, B]]] + [B, [B, [B, A]]] \\
&\quad \left. + [A, [B, [B, A]]] - [B, [A, [A, B]]] \right) \\
&= \frac{1}{48} [A, [B, [B, A]]] - \frac{1}{48} [B, [A, [A, B]]] = \frac{1}{24} [A, [B, [B, A]]].
\end{aligned}$$

The Jacobi identity

$$[A, [B, C]] + [B, [C, A]] + [C, [A, B]] = 0$$

was used in the last step for  $c_4$ .

# Appendix F: The Logarithm of a Matrix

Exponentials of square matrices  $\underline{G}$ ,  $\underline{M} = \exp \underline{G} = \sum_{n=0}^{\infty} \underline{G}^n / n!$ , are frequently used for the representation of symmetry transformations. Indeed, the properties of continuous symmetry transformations are often discussed in terms of their first order approximations  $\underline{1} + \underline{G}$ , where it is assumed that continuity of the symmetries allows for parameter choices such that  $\max |G_{ij}| \ll 1$ . It is therefore of interest that the logarithm  $\underline{G} = \ln \underline{M}$  of invertible square matrices can also be defined, although the existence of  $\underline{G}$  does not imply that it can be chosen to satisfy  $\max |G_{ij}| \ll 1$  for  $\underline{M}$  close to the unit matrix, see below.

Suppose  $\underline{M}$  is a complex invertible square matrix which is related to its Jordan canonical form through

$$\underline{M} = \underline{T} \cdot \oplus_n \underline{J}_n \cdot \underline{T}^{-1}.$$

Each of the smaller square matrices  $\underline{J}_n$  has the form

$$\underline{J} = \lambda \underline{1} \tag{F.1}$$

or the form

$$\underline{J} = \begin{pmatrix} \lambda & 1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & \lambda & 1 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & \lambda & 1 & 0 \\ 0 & 0 & 0 & 0 & \dots & 0 & \lambda & 1 \\ 0 & 0 & 0 & 0 & \dots & 0 & 0 & \lambda \end{pmatrix}, \tag{F.2}$$

and  $\det(\underline{M}) \neq 0$  implies that none of the eigenvalues  $\lambda$  can vanish.

In the case (F.1) we have

$$\underline{J} = \exp(\ln \lambda \underline{1}), \quad \ln \underline{J} = \ln \lambda \underline{1}.$$

However, it is also possible to construct the logarithm of a Jordan block matrix (F.2). The direct sum of the logarithms of all the matrices  $\underline{J}_n$  then yields the logarithm of the matrix  $\underline{M}$ ,

$$\underline{M} = \exp(\underline{T} \cdot \oplus_n \ln \underline{J}_n \cdot \underline{T}^{-1}), \quad \ln \underline{M} = \underline{T} \cdot \oplus_n \ln \underline{J}_n \cdot \underline{T}^{-1}.$$

Suppose the Jordan matrix (F.2) is a  $(\nu + 1) \times (\nu + 1)$  matrix. We define  $(\nu + 1) \times (\nu + 1)$  matrices  $\underline{N}_n$ ,  $0 \leq n \leq \nu$ , according to  $(\underline{N}_n)_{ij} = \delta_{i+n,j}$ , i.e.  $\underline{N}_0$  is the  $(\nu + 1) \times (\nu + 1)$  unit matrix and  $\underline{N}_{1 \leq n \leq \nu}$  has non-vanishing entries 1 only in the  $n$ -th diagonal above the main diagonal. These matrices satisfy the multiplication law  $\underline{N}_m \cdot \underline{N}_n = \Theta(\nu - m - n + \epsilon) \underline{N}_{m+n}$ , which also implies  $\underline{N}_n = (\underline{N}_1)^n$ .

Each  $(\nu + 1) \times (\nu + 1)$  Jordan block can be written as  $\underline{J} = \lambda \underline{N}_0 + \underline{N}_1$ , and its logarithm can be defined through

$$\begin{aligned} \underline{X} = \ln \underline{J} &= \begin{pmatrix} \ln \lambda & \lambda^{-1} & -\lambda^{-2}/2 & \lambda^{-3}/3 & \dots & (-)^{\nu-1} \lambda^{-\nu}/\nu \\ 0 & \ln \lambda & \lambda^{-1} & -\lambda^{-2}/2 & \dots & (-)^{\nu-2} \lambda^{-(\nu-1)}/(\nu-1) \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \dots & -\lambda^{-2}/2 \\ 0 & 0 & 0 & 0 & \dots & \lambda^{-1} \\ 0 & 0 & 0 & 0 & \dots & \ln \lambda \end{pmatrix} \\ &= \underline{N}_0 \ln \lambda - \sum_{n=1}^{\nu} \frac{(-\lambda)^{-n}}{n} \underline{N}_n. \end{aligned} \quad (\text{F.3})$$

We can prove  $\exp(\underline{X}) = \underline{J}$  in the following way. The  $N$ -th power of  $\underline{X}$  is (here  $0 < \epsilon < 1$  is introduced to avoid the ambiguity of the  $\Theta$  function at 0)

$$\begin{aligned} \underline{X}^N &= \underline{N}_0 (\ln \lambda)^N + (-)^N \sum_{1 \leq n_1, n_2, \dots, n_N}^{\nu+1-N} \Theta \left( \nu + \epsilon - \sum_{i=1}^N n_i \right) \\ &\quad \times \frac{(-\lambda)^{-n_1 - n_2 - \dots - n_N}}{n_1 \cdot n_2 \cdot \dots \cdot n_N} \underline{N}_{n_1 + n_2 + \dots + n_N} \\ &\quad - (-)^N N \ln \lambda \sum_{1 \leq n_1, n_2, \dots, n_{N-1}}^{\nu+2-N} \Theta \left( \nu + \epsilon - \sum_{i=1}^{N-1} n_i \right) \\ &\quad \times \frac{(-\lambda)^{-n_1 - n_2 - \dots - n_{N-1}}}{n_1 \cdot n_2 \cdot \dots \cdot n_{N-1}} \underline{N}_{n_1 + n_2 + \dots + n_{N-1}} \end{aligned}$$

$$\begin{aligned}
 &+ (-1)^N \binom{N}{2} (\ln \lambda)^2 \\
 &\times \sum_{1 \leq n_1, n_2, \dots, n_{N-2}}^{\nu+3-N} \Theta \left( \nu + \epsilon - \sum_{i=1}^{N-2} n_i \right) \\
 &\times \frac{(-\lambda)^{-n_1-n_2-\dots-n_{N-2}}}{n_1 \cdot n_2 \cdot \dots \cdot n_{N-2}} \underline{N}_{n_1+n_2+\dots+n_{N-2}} + \dots \\
 &- N (\ln \lambda)^{N-1} \sum_{n=1}^{\nu} \frac{(-\lambda)^{-n}}{n} \underline{N}_n.
 \end{aligned}$$

We can combine terms in the form

$$\begin{aligned}
 \underline{X}^N &= \underline{N}_0 (\ln \lambda)^N + \sum_{m=1}^N (-1)^m \binom{N}{m} (\ln \lambda)^{N-m} \\
 &\times \sum_{1 \leq n_1, n_2, \dots, n_m}^{\nu+1-m} \Theta \left( \nu + \epsilon - \sum_{i=1}^m n_i \right) \frac{(-\lambda)^{-n_1-n_2-\dots-n_m}}{n_1 \cdot n_2 \cdot \dots \cdot n_m} \underline{N}_{n_1+n_2+\dots+n_m} \\
 &= \underline{N}_0 (\ln \lambda)^N + \sum_{M=1}^{\nu} (-\lambda)^{-M} \underline{N}_M \sum_{m=1}^{\min(N,M)} (-1)^m \binom{N}{m} (\ln \lambda)^{N-m} \\
 &\times \sum_{\substack{1 \leq n_1, n_2, \dots, n_m \\ n_1+n_2+\dots+n_m=M}}^{M+1-m} \frac{1}{n_1 \cdot n_2 \cdot \dots \cdot n_m}.
 \end{aligned}$$

This is after isolation of the term with  $M = 1$  in the sum,

$$\begin{aligned}
 \underline{X}^N &= \underline{N}_0 (\ln \lambda)^N + N \frac{(\ln \lambda)^{N-1}}{\lambda} \underline{N}_1 + \Theta(\nu - 2 + \epsilon) \\
 &\times \sum_{M=2}^{\nu} (-\lambda)^{-M} \underline{N}_M \left( \sum_{m=1}^{\min(N,M)} (-1)^m \binom{N}{m} (\ln \lambda)^{N-m} \right. \\
 &\times \left. \sum_{\substack{1 \leq n_1, n_2, \dots, n_m \\ n_1+n_2+\dots+n_m=M}}^{M+1-m} \frac{1}{n_1 \cdot n_2 \cdot \dots \cdot n_m} \right).
 \end{aligned}$$

Only the first two terms survive in

$$\exp(\underline{X}) = \underline{1} + \sum_{N=1}^{\infty} \frac{\underline{X}^N}{N!} = \lambda \underline{N}_0 + \underline{N}_1 = \underline{J}$$

because the sum over  $N$  in the term of order  $M$  reduces to

$$\sum_{N=m}^{\infty} \frac{(\ln \lambda)^{N-m}}{(N-m)!} = \lambda,$$

and the remaining sums yield for  $M \geq 1$

$$\begin{aligned} & \sum_{m=1}^M \frac{(-)^m}{m!} \sum_{\substack{1 \leq n_1, n_2, \dots, n_m \\ n_1 + n_2 + \dots + n_m = M}}^{M+1-m} \frac{1}{n_1 \cdot n_2 \cdot \dots \cdot n_m} \\ &= \frac{1}{2\pi i} \oint_{|z|<1} dz \sum_{m=1}^M \frac{(-)^m}{m!} \sum_{n_1, n_2, \dots, n_m=1}^{\infty} \frac{z^{n_1+n_2+\dots+n_m-M-1}}{n_1 \cdot n_2 \cdot \dots \cdot n_m} \\ &= \frac{1}{2\pi i} \oint_{|z|<1} dz \sum_{m=1}^{\infty} \frac{(-)^m}{m!} \sum_{n_1, n_2, \dots, n_m=1}^{\infty} \frac{z^{n_1+n_2+\dots+n_m-M-1}}{n_1 \cdot n_2 \cdot \dots \cdot n_m} \\ &= \frac{1}{2\pi i} \oint_{|z|<1} dz \sum_{m=1}^{\infty} \frac{(-)^m}{m!} \left( \sum_{n=1}^{\infty} \frac{z^n}{n} \right)^m z^{-M-1} \\ &= \frac{1}{2\pi i} \oint_{|z|<1} dz \sum_{m=1}^{\infty} \frac{[\ln(1-z)]^m}{m!} z^{-M-1} \\ &= \frac{1}{2\pi i} \oint_{|z|<1} dz (z^{-M-1} - z^{-M}) = -\delta_{M,1}. \end{aligned}$$

Equation (F.3) is a special case of a general procedure to define functions  $\underline{M} \rightarrow f(\underline{M})$  of square matrices [16], and for every  $n \in \mathbb{Z}$ , the matrix  $\underline{X} + 2\pi i n \underline{N}_0$  is also a logarithm of  $\underline{J}$ .

A glance at (F.3) tells us that we should avoid matrices with Jordan blocks in their eigenvalue decomposition if we want to find logarithms with the property  $\max |(\ln \underline{M})_{ij}| \ll 1$  for  $\max |M_{ij} - \delta_{ij}| \ll 1$ . This can be achieved if we use hermitian and unitary matrices, and if  $\underline{M}$  does not satisfy this condition, we can use its polar decomposition

$$\underline{M} = \underline{H} \cdot \underline{U} = (\underline{M} \cdot \underline{M}^+)^{1/2} \cdot [(\underline{M} \cdot \underline{M}^+)^{-1/2} \cdot \underline{M}] \tag{F.4}$$

in terms of a hermitian and a unitary factor, or a symmetric and an orthogonal factor if  $\underline{M}$  is real. The factors will then have logarithms with small matrix elements if  $\underline{M}$  is close to the unit matrix, i.e. the analysis of continuous symmetries in finite-dimensional vector spaces eventually requires the analysis of up to two first order transformations  $\underline{1} + \ln \underline{H}$  and  $\underline{1} + \ln \underline{U}$ . This is the case e.g. for Lorentz transformations, where  $\underline{H}$  is the pure boost part and  $\underline{U}$  is the rotation.

# Appendix G: Dirac $\gamma$ matrices

It is useful for the understanding and explicit construction of  $\gamma$  matrices to discuss their properties in a general number  $d$  of spacetime dimensions.  $\gamma$  matrices in more than four spacetime dimensions are regularly used in theories which hypothesize the existence of extra spacetime dimensions. On the other hand, variants of the Dirac equation in two space dimensions or three spacetime dimensions have also become relevant in materials science for the description of electrons in Graphene and other two-dimensional materials.

## $\gamma$ -matrices in $d$ dimensions

The condition (21.35),  $\{\gamma_\mu, \gamma_\nu\} = -2\eta_{\mu\nu}$ , implies that any product of  $n$  gamma coefficients  $\gamma_\alpha \cdot \gamma_\beta \cdot \dots \cdot \gamma_\omega$  can be reduced to a product of  $n - 2$  coefficients if two indices have the same value. We can also re-order any product such that the indices have increasing values. These observations imply that the  $d$  coefficients  $\gamma_\mu$  can produce at most  $2^d$  linearly independent combinations

$$\mathbf{1}, \gamma_0, \gamma_1, \dots, \gamma_{d-1}, \gamma_0 \cdot \gamma_1, \gamma_0 \cdot \gamma_2, \dots, \gamma_0 \cdot \gamma_1 \cdot \dots \cdot \gamma_{d-1}. \tag{G.1}$$

We are actually interested in matrix representations of the algebra generated by (21.35), and consider the coefficients  $\gamma^\mu$  and the objects in (G.1) as matrices in the following. We first discuss the case that  $d$  is an *even number of spacetime dimensions*, and we define multi-indices  $J$  through

$$\Gamma_J = \gamma_{\mu_1} \cdot \gamma_{\mu_2} \cdot \dots \cdot \gamma_{\mu_n}, \quad \mu_1 < \mu_2 < \dots < \mu_n, \quad n(J) = n. \tag{G.2}$$

It is easy to prove that

$$\text{tr}(\Gamma_J) = 0. \tag{G.3}$$

For even  $n(J)$  this follows from the anti-commutativity of the  $\gamma$ -matrices and the cyclic invariance of the trace. For odd  $n(J)$  this follows from the fact that there is at least one  $\gamma$ -matrix not contained in  $\Gamma_J$ , e.g.  $\gamma_1$ , and therefore

$$\text{tr}(\Gamma_J) = -\text{tr}(\gamma_1^2 \cdot \Gamma_J) = -\text{tr}(\gamma_1 \cdot \Gamma_J \cdot \gamma_1) = \text{tr}(\gamma_1^2 \cdot \Gamma_J) = -\text{tr}(\Gamma_J) = 0.$$

The product  $\Gamma_I \cdot \Gamma_J$  reduces either to a  $\Gamma$ -matrix  $\Gamma_K$  if  $I \neq J$ , or otherwise

$$\Gamma_I^2 = \pm \mathbf{1},$$

and this implies orthogonality of all the  $\Gamma$ -matrices and  $\mathbf{1}$ ,

$$\text{tr}(\Gamma_I \cdot \Gamma_J) \propto \delta_{IJ}.$$

For *even number of spacetime dimensions*  $d$  this implies that all the  $2^d$  matrices in (G.1) are indeed linearly independent, and therefore a minimal matrix representation of (21.35) requires at least  $(2^{d/2} \times 2^{d/2})$ -matrices. We will see by explicit construction that such a representation exists, and because  $2^{d/2}$  is the minimal dimension, the representation must be irreducible, i.e. cannot split into smaller matrices acting in spaces of lower dimensions. The representation also turns out to be unique up to similarity transformations

$$\gamma_\mu \rightarrow \gamma'_\mu = A \cdot \gamma_\mu \cdot A^{-1}.$$

For *odd number of spacetime dimensions*  $d$ , we also define the matrices  $\Gamma_J$  according to (G.1), but now the previous proof of  $\text{tr}(\Gamma_J) = 0$  only goes through for all the matrices  $\Gamma_J$  *except for the last matrix in the list*,

$$\Gamma_{0,1,\dots,d-1} = \gamma_0 \cdot \gamma_1 \cdot \dots \cdot \gamma_{d-1}.$$

For odd  $d$ , this matrix contains an odd number of  $\gamma$ -matrices, and it contains all  $\gamma$ -matrices, such that the previous proof of vanishing trace for odd  $n(J)$  does not go through for this particular matrix. Furthermore, this matrix has the properties

$$[\Gamma_{0,1,\dots,d-1}, \Gamma_J] = 0, \tag{G.4}$$

$$\Gamma_{0,1,\dots,d-1}^2 = (-1)^{(d+2)(d-1)/2} \mathbf{1} = (-1)^{(d-1)/2} \mathbf{1}. \tag{G.5}$$

Commutativity with all other matrices implies that in every irreducible representation

$$\Gamma_{0,1,\dots,d-1} = \pm (-1)^{(d-1)/4} \mathbf{1}, \tag{G.6}$$

see the following subsection for the proof.

This also implies that every product  $\Gamma_J$  of  $n(J) \geq (d + 1)/2$   $\gamma$  matrices is up to a numerical factor a product  $\Gamma_I$  of  $n(I) = d - n(J) \leq (d - 1)/2$   $\gamma$  matrices,

$$\begin{aligned} \left[ \Gamma_J \right]_{n(J) \geq (d+1)/2} &= \left[ \mathbf{1} \cdot \Gamma_J \right]_{n(J) \geq (d+1)/2} \propto \left[ \Gamma_{0,1,\dots,d-1} \cdot \Gamma_J \right]_{n(J) \geq (d+1)/2} \\ &\propto \left[ \Gamma_I \right]_{n(I) \leq (d-1)/2}. \end{aligned}$$

Therefore there are only  $2^{d-1}$  linearly independent matrices in (G.1) for odd  $d$ , and the minimal possible dimension of the representation is only  $2^{(d-1)/2}$ . The explicit construction later on confirms that the minimal dimension also works for odd number of spacetime dimensions. There are two different equivalence classes of matrix representations with dimension  $2^{(d-1)/2}$ .

We can summarize the results on the dimensions of  $\gamma$  matrices in  $d$  space(-time) dimensions by the statement the irreducible representations of the Dirac algebra are provided by  $2^{\lfloor d/2 \rfloor} \times 2^{\lfloor d/2 \rfloor}$  matrices, where the floor function in the exponents rounds to the next lowest integer and is also often written in terms of Gauss brackets:  $\lfloor d/2 \rfloor \equiv [d/2]_G = d/2$  if  $d$  is even,  $\lfloor d/2 \rfloor \equiv [d/2]_G = (d - 1)/2$  if  $d$  is odd.

### Proof that in irreducible representations $\Gamma_{0,1,\dots,d-1} \propto \mathbf{1}$ for odd spacetime dimension $d$

$\Gamma_{0,1,\dots,d-1}$  commutes with all  $\Gamma_J$ . Suppose that we have an irreducible matrix representation of (G.1) in a vector space  $V$  of dimension  $\dim V$ . If  $\lambda$  is an eigenvalue of  $\Gamma_{0,1,\dots,d-1} \propto \mathbf{1}$ ,

$$\det(\Gamma_{0,1,\dots,d-1} - \lambda \mathbf{1}) = 0,$$

we have

$$\dim\left((\Gamma_{0,1,\dots,d-1} - \lambda \mathbf{1}) \cdot V\right) \leq \dim V - 1,$$

and

$$\Gamma_J \cdot (\Gamma_{0,1,\dots,d-1} - \lambda \mathbf{1}) \cdot V = (\Gamma_{0,1,\dots,d-1} - \lambda \mathbf{1}) \cdot \Gamma_J \cdot V.$$

The last equation would imply that  $(\Gamma_{0,1,\dots,d-1} - \lambda \mathbf{1}) \cdot V$ , if non-empty, would be an invariant subspace under the action of the  $\gamma$ -matrices, in contradiction to the irreducibility of  $V$ . Therefore we must have

$$(\Gamma_{0,1,\dots,d-1} - \lambda \mathbf{1}) \cdot V = \emptyset, \quad \Gamma_{0,1,\dots,d-1} = \lambda \mathbf{1}$$

in every irreducible representation. Equation (G.5) tells us that

$$\lambda = \pm(-)^{(d-1)/4}.$$

The proof is simply an adaptation of the proof of Schur's lemma from group theory.

## Recursive construction of $\gamma$ -matrices in different dimensions

We will use the following conventions for the explicit construction of  $\gamma$ -matrices: Up to similarity transformations, the  $\gamma$ -matrices in *two spacetime dimensions* are

$$\gamma_0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma_1 = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \quad (\text{G.7})$$

For the recursive construction in higher dimensions  $d \geq 3$  we now assume that  $\gamma_\mu$ ,  $0 \leq \mu \leq d-2$ , are  $\gamma$ -matrices in  $d-1$  dimensions.

For the construction of  $\gamma$ -matrices in an *odd number  $d$  of spacetime dimensions* there are two inequivalent choices,

$$\begin{aligned} \Gamma_0 &= \pm i^{(d-3)/2} \gamma_0 \gamma_1 \dots \gamma_{d-2} = \pm \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \Gamma_i = \gamma_i, \quad 1 \leq i \leq d-2, \\ \Gamma_{d-1} &= -i\gamma_0. \end{aligned} \quad (\text{G.8})$$

For the construction of  $\gamma$ -matrices in an *even number  $d \geq 4$  of spacetime dimensions* there is only one equivalence class of representations,

$$\begin{aligned} \Gamma_0 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \Gamma_i = \begin{pmatrix} 0 & -\gamma_0 \gamma_i \\ \gamma_0 \gamma_i & 0 \end{pmatrix}, \quad 1 \leq i \leq d-2, \\ \Gamma_{d-1} &= \begin{pmatrix} 0 & -\gamma_0 \\ \gamma_0 & 0 \end{pmatrix}. \end{aligned} \quad (\text{G.9})$$

Note that it does not matter from which of the two possible representations  $\pm\gamma_0$  in the odd number  $d-1$  of lower dimensions we start since  $\Gamma_0$  intertwines the two possibilities,

$$\Gamma_0 \Gamma_i \Gamma_0 = -\Gamma_i, \quad 1 \leq i \leq d-1.$$

The possibility of similarity transformations implies that there are infinitely many equivalent possibilities to construct these bases of  $\gamma$ -matrices. The construction described here was motivated from the desire to have Weyl bases (i.e. all  $\gamma^\mu$  have

only off-diagonal non-vanishing ( $2^{(d/2)-1} \times 2^{(d/2)-1}$ ) blocks) in even dimensions, and to have the next best solution, *viz.* Dirac bases (i.e.  $\gamma^0 = \pm \text{diag}(\mathbf{1}, -\mathbf{1})$ , all  $\gamma^i$  like in a Weyl basis), in odd dimensions. Note that all the representations (G.8) and (G.9) of the  $\gamma$ -matrices in odd or even dimensions fulfill

$$\gamma_0^+ = \gamma_0, \quad \gamma_i^+ = -\gamma_i,$$

or equivalently

$$\gamma_\mu^+ = \gamma_0 \gamma_\mu \gamma_0. \tag{G.10}$$

Every set of  $\gamma$ -matrices is equivalent to a set satisfying equation (G.10). We will prove this in the following subsection.

### Proof that every set of $\gamma$ -matrices is equivalent to a set which satisfies equation (G.10)

In this section we do not use summation convention but spell out all summations explicitly.

We define  $2^{\lfloor d/2 \rfloor} \times 2^{\lfloor d/2 \rfloor}$  matrices  $X_0 = \gamma_0, X_i = i\gamma_i$ ,

$$\{X_\mu, X_\nu\} = 2\delta_{\mu\nu}$$

and prove that the matrices  $X_\mu$  are equivalent to a set of unitary matrices  $Y_\mu$ . Since the matrices  $Y_\mu$  also satisfy  $Y_\mu^{-1} = Y_\mu$ , unitarity also implies hermiticity of  $Y_\mu$ . We use the abbreviation  $N = 2^{\lfloor d/2 \rfloor}$ , and consider the set  $\mathbb{S}$  of  $N \times N$  matrices

$$\mathbf{1}, \quad X_I = X_{\mu_1} \cdot \dots \cdot X_{\mu_n}, \quad n \leq \hat{n} = \begin{cases} d, & d \text{ even} \\ \frac{d-1}{2}, & d \text{ odd} \end{cases}$$

This set does not form a group, but only a group modulo  $\mathbb{Z}_2$ . But this is sufficient for the standard argument for equivalence to a set of unitary matrices.

The  $N \times N$  matrix

$$H = \mathbf{1} + \sum_I X_I^+ \cdot X_I = H^+$$

is invariant under right translations in the set  $\mathbb{S}$  (i.e. right multiplication of all elements by some fixed element  $Z$ ), because that just permutes the elements, up to possible additional minus signs which cancel in  $H$ ,

$$H = Z^+ \cdot Z + \sum_I (X_I \cdot Z)^+ \cdot (X_I \cdot Z).$$

$H$  also has  $N$  positive eigenvalues, because

$$H \cdot \psi_\alpha = h_\alpha \psi_\alpha, \quad \psi_\alpha^\dagger \cdot \psi_\beta = \delta_{\alpha\beta}, \quad (\text{G.11})$$

implies

$$h_\alpha = \psi_\alpha^\dagger \cdot H \cdot \psi_\alpha = 1 + \sum_I |X_I \cdot \psi_\alpha|^2 > 0. \quad (\text{G.12})$$

If we define the matrix  $\Psi$  with columns  $\psi_\alpha$ , equations (G.11) and (G.12) imply

$$\text{diag}(h_1, \dots, h_N) = \Psi^\dagger \cdot H \cdot \Psi, \quad H = \Psi \cdot \text{diag}(h_1, \dots, h_N) \cdot \Psi^\dagger.$$

Now define

$$Y_\mu = \Psi \cdot \text{diag}(\sqrt{h_1}, \dots, \sqrt{h_N}) \cdot \Psi^\dagger \cdot X_\mu \cdot (\Psi \cdot \text{diag}(\sqrt{h_1}, \dots, \sqrt{h_N}) \cdot \Psi^\dagger)^{-1}.$$

These matrices are indeed unitary,

$$\begin{aligned} Y_\mu^\dagger \cdot Y_\mu &= \left( \Psi \cdot \text{diag}(\sqrt{h_1}, \dots, \sqrt{h_N}) \cdot \Psi^\dagger \right)^{-1} \cdot X_\mu^\dagger \\ &\quad \times \left( \Psi \cdot \text{diag}(\sqrt{h_1}, \dots, \sqrt{h_N}) \cdot \Psi^\dagger \right)^2 \cdot X_\mu \\ &\quad \times \left( \Psi \cdot \text{diag}(\sqrt{h_1}, \dots, \sqrt{h_N}) \cdot \Psi^\dagger \right)^{-1} \\ &= \left( \Psi \cdot \text{diag}(\sqrt{h_1}, \dots, \sqrt{h_N}) \cdot \Psi^\dagger \right)^{-1} \cdot X_\mu^\dagger \cdot H \cdot X_\mu \\ &\quad \times \left( \Psi \cdot \text{diag}(\sqrt{h_1}, \dots, \sqrt{h_N}) \cdot \Psi^\dagger \right)^{-1} \\ &= \left( \Psi \cdot \text{diag}(\sqrt{h_1}, \dots, \sqrt{h_N}) \cdot \Psi^\dagger \right)^{-1} \\ &\quad \times [X_\mu^\dagger \cdot X_\mu + \sum_I (Z_I \cdot X_\mu)^\dagger \cdot (Z_I \cdot X_\mu)] \\ &\quad \times \left( \Psi \cdot \text{diag}(\sqrt{h_1}, \dots, \sqrt{h_N}) \cdot \Psi^\dagger \right)^{-1} \\ &= \left( \Psi \cdot \text{diag}(\sqrt{h_1}, \dots, \sqrt{h_N}) \cdot \Psi^\dagger \right)^{-1} \cdot H \\ &\quad \times \left( \Psi \cdot \text{diag}(\sqrt{h_1}, \dots, \sqrt{h_N}) \cdot \Psi^\dagger \right)^{-1} = \mathbf{1}, \end{aligned}$$

which concludes the proof of equivalence of the matrices  $X_\mu$  to a set of matrices  $Y_\mu$  which are both unitary and hermitian.

Equivalence of the  $\gamma$  matrices to hermitian or anti-hermitian matrices also implies that every reducible representation of  $\gamma$  matrices is fully reducible.

### Uniqueness theorem for $\gamma$ matrices

Every irreducible matrix representation of the algebra generated by (21.35) is equivalent to one of the representations constructed in the previous section.

We first consider the case of *even number of dimensions*  $d$ . The theorem says that in this case every irreducible matrix representation of (21.35) is equivalent to the representation in terms of  $2^{d/2} \times 2^{d/2}$  constructed in equation (G.9).

*Proof.* Suppose the  $N_1 \times N_1$  matrices  $\gamma_{1,\mu}$  and the  $N_2 \times N_2$  matrices  $\gamma_{2,\mu}$ ,  $0 \leq \mu \leq d - 1$ , are two sets of matrices which satisfy the conditions (21.35).  $V_1$  is the  $N_1$ -dimensional vector space in which the matrices  $\gamma_{1,\mu}$  act. We use the representations from the previous section, equation (G.9), for the matrices  $\gamma_{2,\mu}$ . This implies  $N_1 \geq N_2 = 2^{d/2}$ .

We denote the components of the matrices  $\gamma_{1,\mu}$  and  $\gamma_{2,\mu}$  with  $\gamma_{1,\mu}{}^a{}_b$  and  $\gamma_{2,\mu}{}^\alpha{}_\beta$ , respectively, and define again multi-indices  $J$  for the two sets of  $\gamma$  matrices (cf. equation (G.2)),

$$\Gamma_{r,J} = \gamma_{r,\mu_1} \cdot \gamma_{r,\mu_2} \cdot \dots \cdot \gamma_{r,\mu_n}, \quad 1 \leq r \leq 2, \quad \mu_1 < \mu_2 < \dots < \mu_n, \quad n(J) = n.$$

The squares of these matrices satisfy

$$\Gamma_{r,J}^2 = \pm \mathbf{1} = s_J \mathbf{1}, \tag{G.13}$$

where the sign factor

$$s_J = (-1)^{n(I)[n(I)+1]/2} \eta_{\mu_1 \mu_1} \tag{G.14}$$

arises as the product of the factor  $(-1)^{n(I)[n(I)-1]/2}$  from the permutations of  $\gamma$  matrices times a factor  $(-1)^{n(I)}$  from the sign on the right hand side of (21.35). Only  $\eta_{\mu_1 \mu_1}$  appears on the right hand side of (G.14) because we have only one timelike direction. For the case of general spacetime signature one could simply include the product  $\eta_{\mu_1 \mu_1} \eta_{\mu_2 \mu_2} \dots \eta_{\mu_n \mu_n}$ .

The results from the previous section for even  $d$  tell us that a set  $\Gamma_{r,J}$  with fixed  $r$ , after augmentation with the  $N_r \times N_r$  unit matrix  $\Gamma_{r,0} = \mathbf{1}$ , contains  $2^d$  linearly independent matrices.

We define the  $N_1 \cdot N_2$  different  $N_1 \times N_2$  matrices  $E_a^\alpha$  with components

$$(E_a^\alpha)^b{}_\beta = \delta_a{}^b \delta^\alpha{}_\beta.$$

We use these matrices to form the  $N_1 \times N_2$  matrices

$$\Omega_a^\alpha = E_a^\alpha + \sum_J s_J \Gamma_{1,J} \cdot E_a^\alpha \cdot \Gamma_{2,J},$$

i.e. in components,

$$(\Omega_a^\alpha)^b{}_\beta = \delta_a^b \delta^\alpha{}_\beta + \sum_J s_J (\Gamma_{1,J})^b{}_a (\Gamma_{2,J})^\alpha{}_\beta. \quad (\text{G.15})$$

Suppose  $I \neq J$ . The conditions (21.35) imply that there is always a multi-index  $K \neq I$  such that

$$\Gamma_{r,I} \cdot \Gamma_{r,J} = \pm \Gamma_{r,K},$$

and inversion of this equation yields

$$s_I s_J \Gamma_{r,J} \cdot \Gamma_{r,I} = \pm s_K \Gamma_{r,K}.$$

This implies

$$\begin{aligned} \Gamma_{1,I} \cdot \Omega_a^\alpha &= \Gamma_{1,I} \cdot E_a^\alpha + E_a^\alpha \cdot \Gamma_{2,I} + \sum_{J \neq I} s_J \Gamma_{1,I} \cdot \Gamma_{1,J} \cdot E_a^\alpha \cdot \Gamma_{2,J} \\ &= \left( s_I \Gamma_{1,I} \cdot E_a^\alpha \cdot \Gamma_{2,I} + E_a^\alpha \right. \\ &\quad \left. + \sum_{J \neq I} s_I s_J \Gamma_{1,I} \cdot \Gamma_{1,J} \cdot E_a^\alpha \cdot \Gamma_{2,J} \cdot \Gamma_{2,I} \right) \cdot \Gamma_{2,I} \\ &= \left( s_I \Gamma_{1,I} \cdot E_a^\alpha \cdot \Gamma_{2,I} + E_a^\alpha + \sum_{K \neq I} s_K \Gamma_{1,K} \cdot E_a^\alpha \cdot \Gamma_{2,K} \right) \cdot \Gamma_{2,I} \\ &= \Omega_a^\alpha \cdot \Gamma_{2,I}. \end{aligned} \quad (\text{G.16})$$

We know that the matrices (G.15) are not null matrices,  $\Omega_a^\alpha \neq \mathbf{0}$ , because we know that the  $2^d$  matrices  $\{\mathbf{1}, \Gamma_{2,J}\}$  are linearly independent,

$$\delta_a^b \mathbf{1} + \sum_J s_J (\Gamma_{1,J})^b{}_a \Gamma_{2,J} \neq 0.$$

This implies that the  $N_1$ -dimensional vector space  $V_1$  with basis vectors  $e_{1,b}$ ,  $1 \leq b \leq N_1$ , contains non-vanishing sets of  $N_2 = 2^{d/2} \leq N_1$  basis vectors

$$e_{1,\beta} = e_{1,b} (\Omega_a^\alpha)^b{}_\beta, \quad 1 \leq \beta \leq 2^{d/2} \leq N_1,$$

which are invariant under the action of the  $\gamma$  matrices,

$$e_{1,b}(\gamma_{1,\mu})^b c(\Omega_a^\alpha)^c \delta = e_{1,b}(\Omega_a^\alpha)^b \beta(\gamma_{2,\mu})^\beta \delta.$$

Therefore the representation of  $\gamma$  matrices in  $V_1$  is either reducible into invariant subspaces of dimension  $2^{d/2}$ , or we have  $N_1 = 2^{d/2}$ . In the latter case we must have

$$\det(\Omega_a^\alpha) \neq 0,$$

because representations spaces of dimension  $2^{d/2}$  are irreducible, and therefore

$$\gamma_{1,\mu} = \Omega_a^\alpha \cdot \gamma_{2,\mu} \cdot (\Omega_a^\alpha)^{-1}$$

is equivalent to the representation from the previous section for even  $d$ . Thus concludes the proof for even  $d$ .

For *odd*  $d$  we observe that the matrices  $\gamma_\mu, 0 \leq \mu \leq d-2$ , form a set of  $\gamma$  matrices for a  $(d-1)$ -dimensional Minkowski space, which according to the previous result is either reducible or equivalent to the corresponding representation (G.9) from the previous section. However, using those matrices, the missing matrix  $\gamma_{d-1}$  can easily be constructed according to the prescription

$$\gamma_{d-1} = \pm(-)^{(d-1)(d-2)/4} \gamma_0 \cdot \gamma_1 \cdot \dots \cdot \gamma_{d-2}. \tag{G.17}$$

Now assume that the matrices  $\gamma_\mu, 0 \leq \mu \leq d-2$ , are  $2^{(d-1)/2} \times 2^{(d-1)/2}$  matrices, i.e. they form an *irreducible* representation of  $\gamma$  matrices for a  $(d-1)$ -dimensional Minkowski space. In that case completeness of the set

$$\Gamma_J = \gamma_{\mu_1} \cdot \gamma_{\mu_2} \cdot \dots \cdot \gamma_{\mu_n}, \quad 0 \leq \mu_1 < \mu_2 < \dots < \mu_n \leq d-2 \tag{G.18}$$

in  $GL(2^{(d-1)/2})$  implies that (G.17) are the only options for the construction of  $\gamma_{d-1}$ . Completeness of the set (G.18) also implies that the two options for the sign in (G.17) correspond to two inequivalent representations.

On the other hand, if the matrices  $\gamma_\mu, 0 \leq \mu \leq d-2$ , form a *reducible* representation of  $\gamma$  matrices for a  $(d-1)$ -dimensional Minkowski space, they must be equivalent to matrices with irreducible  $2^{(d-1)/2} \times 2^{(d-1)/2}$  matrices  $\hat{\gamma}_\mu, 0 \leq \mu \leq d-2$ , in diagonal blocks. Then one can easily prove from the anti-commutation relations and the completeness of the set

$$\hat{\Gamma}_J = \hat{\gamma}_{\mu_1} \cdot \hat{\gamma}_{\mu_2} \cdot \dots \cdot \hat{\gamma}_{\mu_n}, \quad 0 \leq \mu_1 < \mu_2 < \dots < \mu_n \leq d-2$$

in  $2^{(d-1)/2}$ -dimensional subspaces that the matrix  $\gamma_{d-1}$  must consist of  $2^{(d-1)/2} \times 2^{(d-1)/2}$  blocks which are proportional to  $\hat{\gamma}_0 \cdot \hat{\gamma}_1 \cdot \dots \cdot \hat{\gamma}_{d-2}$ . The property  $\gamma_{d-1}^2 = -1$  can then be used to demonstrate that  $\gamma_{d-1}$  must be equivalent to a matrix which only has matrices

$$\hat{\gamma}_{d-1} = \pm(-)^{(d-1)(d-2)/4} \hat{\gamma}_0 \cdot \hat{\gamma}_1 \cdot \dots \cdot \hat{\gamma}_{d-2}$$

in diagonal  $2^{(d-1)/2} \times 2^{(d-1)/2}$  blocks, i.e. a representation of  $\gamma$  matrices for odd number  $d$  of dimensions is either equivalent to one of the two irreducible  $2^{(d-1)/2}$ -dimensional representations distinguished by the sign in (G.17), or it is a reducible representation.

In the recursive construction of  $\gamma$  matrices described above, I separated the two equivalence classes of irreducible representations through the sign of  $\gamma_0$  instead of  $\gamma_{d-1}$ , cf. (G.8). We can cast the sign from  $\gamma_{d-1}$  to  $\gamma_0$  through the similarity transformation

$$\begin{aligned}\gamma_0 &\rightarrow \gamma_0 \cdot \gamma_{d-1} \cdot \gamma_0 \cdot \gamma_0 \cdot \gamma_{d-1} = -\gamma_0, \\ \gamma_{d-1} &\rightarrow \gamma_0 \cdot \gamma_{d-1} \cdot \gamma_{d-1} \cdot \gamma_0 \cdot \gamma_{d-1} = -\gamma_{d-1}, \\ \gamma_i &\rightarrow \gamma_0 \cdot \gamma_{d-1} \cdot \gamma_i \cdot \gamma_0 \cdot \gamma_{d-1} = \gamma_i, \quad 1 \leq i \leq d-2.\end{aligned}$$

## Contraction and trace theorems for $\gamma$ matrices

Here we explicitly refer to four spacetime dimensions again. The generalizations to any number of spacetime dimensions are trivial.

Equation (21.35) implies

$$\gamma^\sigma \gamma_\sigma = -4.$$

The higher order contraction theorems then follow from (21.35) and application of the next lower order contraction theorem, e.g.

$$\begin{aligned}\gamma^\sigma \gamma^\mu \gamma_\sigma &= \{\gamma^\sigma, \gamma^\mu\} \gamma_\sigma - \gamma^\mu \gamma^\sigma \gamma_\sigma = 2\gamma^\mu, \\ \gamma^\sigma \gamma^\mu \gamma^\nu \gamma_\sigma &= 4\eta^{\mu\nu}, \quad \gamma^\sigma \gamma^\mu \gamma^\nu \gamma^\rho \gamma_\sigma = 2\gamma^\rho \gamma^\nu \gamma^\mu.\end{aligned}$$

The trace of a product of an odd number of  $\gamma$  matrices vanishes. The trace of a product of two  $\gamma$  matrices is determined by their basic anti-commutation property,

$$\text{tr}(\gamma_\mu \gamma_\nu) = -4\eta_{\mu\nu}. \quad (\text{G.19})$$

The trace of a product of four  $\gamma$  matrices is easily evaluated using their anti-commutation properties and cyclic invariance of the trace

$$\begin{aligned}\text{tr}(\gamma_\kappa \gamma_\lambda \gamma_\mu \gamma_\nu) &= 8\eta_{\kappa\lambda} \eta_{\mu\nu} - \text{tr}(\gamma_\kappa \gamma_\lambda \gamma_\nu \gamma_\mu) = 8\eta_{\kappa\lambda} \eta_{\mu\nu} - \text{tr}(\gamma_\mu \gamma_\kappa \gamma_\lambda \gamma_\nu) \\ &= 8\eta_{\kappa\lambda} \eta_{\mu\nu} - 8\eta_{\mu\kappa} \eta_{\lambda\nu} + \text{tr}(\gamma_\kappa \gamma_\mu \gamma_\lambda \gamma_\nu) \\ &= 8\eta_{\kappa\lambda} \eta_{\mu\nu} - 8\eta_{\mu\kappa} \eta_{\lambda\nu} + 8\eta_{\mu\lambda} \eta_{\kappa\nu} - \text{tr}(\gamma_\kappa \gamma_\lambda \gamma_\mu \gamma_\nu),\end{aligned}$$

i.e.

$$\mathrm{tr}(\gamma_\kappa \gamma_\lambda \gamma_\mu \gamma_\nu) = 4\eta_{\kappa\lambda} \eta_{\mu\nu} - 4\eta_{\mu\kappa} \eta_{\lambda\nu} + 4\eta_{\mu\lambda} \eta_{\kappa\nu}. \quad (\text{G.20})$$

For yet higher orders we observe

$$\begin{aligned} \mathrm{tr}(\gamma_{\alpha_1} \dots \gamma_{\alpha_{2n}} \gamma_\mu \gamma_\nu) &= -2\eta_{\mu\nu} \mathrm{tr}(\gamma_{\alpha_1} \dots \gamma_{\alpha_{2n}}) - \mathrm{tr}(\gamma_\mu \gamma_{\alpha_1} \dots \gamma_{\alpha_{2n}} \gamma_\nu) \\ &= -2\eta_{\mu\nu} \mathrm{tr}(\gamma_{\alpha_1} \dots \gamma_{\alpha_{2n}}) + \mathrm{tr}(\gamma_{\alpha_1} \gamma_\mu \gamma_{\alpha_2} \dots \gamma_{\alpha_{2n}} \gamma_\nu) \\ &\quad + 2\eta_{\mu\alpha_1} \mathrm{tr}(\gamma_{\alpha_2} \dots \gamma_{\alpha_{2n}} \gamma_\nu) \\ &= -2\eta_{\mu\nu} \mathrm{tr}(\gamma_{\alpha_1} \dots \gamma_{\alpha_{2n}}) - \mathrm{tr}(\gamma_{\alpha_1} \dots \gamma_{\alpha_{2n}} \gamma_\mu \gamma_\nu) \\ &\quad - 2 \sum_{i=1}^{2n} (-)^i \eta_{\mu\alpha_i} \mathrm{tr}(\gamma_{\alpha_1} \dots \gamma_{\alpha_{i-1}} \gamma_{\alpha_{i+1}} \dots \gamma_{\alpha_{2n}} \gamma_\nu), \end{aligned}$$

i.e. we have a recursion relation

$$\begin{aligned} \mathrm{tr}(\gamma_{\alpha_1} \dots \gamma_{\alpha_{2n}} \gamma_\mu \gamma_\nu) &= -\eta_{\mu\nu} \mathrm{tr}(\gamma_{\alpha_1} \dots \gamma_{\alpha_{2n}}) \\ &\quad - \sum_{i=1}^{2n} (-)^i \eta_{\mu\alpha_i} \mathrm{tr}(\gamma_{\alpha_1} \dots \gamma_{\alpha_{i-1}} \gamma_{\alpha_{i+1}} \dots \gamma_{\alpha_{2n}} \gamma_\nu). \end{aligned}$$

This yields for products of six  $\gamma$  matrices

$$\begin{aligned} \mathrm{tr}(\gamma_\rho \gamma_\sigma \gamma_\kappa \gamma_\lambda \gamma_\mu \gamma_\nu) &= -4\eta_{\rho\sigma} \eta_{\kappa\lambda} \eta_{\mu\nu} + 4\eta_{\rho\kappa} \eta_{\sigma\lambda} \eta_{\mu\nu} - 4\eta_{\rho\lambda} \eta_{\kappa\sigma} \eta_{\mu\nu} + 4\eta_{\sigma\kappa} \eta_{\lambda\nu} \eta_{\mu\rho} \\ &\quad - 4\eta_{\sigma\lambda} \eta_{\kappa\nu} \eta_{\mu\rho} + 4\eta_{\sigma\nu} \eta_{\lambda\kappa} \eta_{\mu\rho} - 4\eta_{\rho\kappa} \eta_{\lambda\nu} \eta_{\mu\sigma} + 4\eta_{\rho\lambda} \eta_{\kappa\nu} \eta_{\mu\sigma} \\ &\quad - 4\eta_{\rho\nu} \eta_{\lambda\kappa} \eta_{\mu\sigma} + 4\eta_{\rho\sigma} \eta_{\lambda\nu} \eta_{\mu\kappa} - 4\eta_{\rho\lambda} \eta_{\sigma\nu} \eta_{\mu\kappa} + 4\eta_{\rho\nu} \eta_{\lambda\sigma} \eta_{\mu\kappa} \\ &\quad - 4\eta_{\rho\sigma} \eta_{\kappa\nu} \eta_{\mu\lambda} + 4\eta_{\rho\kappa} \eta_{\sigma\nu} \eta_{\mu\lambda} - 4\eta_{\rho\nu} \eta_{\kappa\sigma} \eta_{\mu\lambda}, \quad (\text{G.21}) \end{aligned}$$

and the trace of the product of eight  $\gamma$  matrices contains 105 terms,

$$\begin{aligned} \mathrm{tr}(\gamma_\alpha \gamma_\beta \gamma_\rho \gamma_\sigma \gamma_\kappa \gamma_\lambda \gamma_\mu \gamma_\nu) &= 4\eta_{\rho\sigma} \eta_{\kappa\lambda} \eta_{\mu\nu} \eta_{\alpha\beta} - 4\eta_{\rho\kappa} \eta_{\sigma\lambda} \eta_{\mu\nu} \eta_{\alpha\beta} + 4\eta_{\rho\lambda} \eta_{\kappa\sigma} \eta_{\mu\nu} \eta_{\alpha\beta} \\ &\quad - 4\eta_{\sigma\kappa} \eta_{\lambda\nu} \eta_{\mu\rho} \eta_{\alpha\beta} + 4\eta_{\sigma\lambda} \eta_{\kappa\nu} \eta_{\mu\rho} \eta_{\alpha\beta} - 4\eta_{\sigma\nu} \eta_{\lambda\kappa} \eta_{\mu\rho} \eta_{\alpha\beta} + 4\eta_{\rho\kappa} \eta_{\lambda\nu} \eta_{\mu\sigma} \eta_{\alpha\beta} \\ &\quad - 4\eta_{\rho\lambda} \eta_{\kappa\nu} \eta_{\mu\sigma} \eta_{\alpha\beta} + 4\eta_{\rho\nu} \eta_{\lambda\kappa} \eta_{\mu\sigma} \eta_{\alpha\beta} - 4\eta_{\rho\sigma} \eta_{\lambda\nu} \eta_{\mu\kappa} \eta_{\alpha\beta} + 4\eta_{\rho\lambda} \eta_{\sigma\nu} \eta_{\mu\kappa} \eta_{\alpha\beta} \\ &\quad - 4\eta_{\rho\nu} \eta_{\lambda\sigma} \eta_{\mu\kappa} \eta_{\alpha\beta} + 4\eta_{\rho\sigma} \eta_{\kappa\nu} \eta_{\mu\lambda} \eta_{\alpha\beta} - 4\eta_{\rho\kappa} \eta_{\sigma\nu} \eta_{\mu\lambda} \eta_{\alpha\beta} + 4\eta_{\rho\nu} \eta_{\kappa\sigma} \eta_{\mu\lambda} \eta_{\alpha\beta} \\ &\quad - 4\eta_{\sigma\kappa} \eta_{\lambda\mu} \eta_{\nu\beta} \eta_{\alpha\rho} + 4\eta_{\sigma\lambda} \eta_{\kappa\mu} \eta_{\nu\beta} \eta_{\alpha\rho} - 4\eta_{\sigma\mu} \eta_{\lambda\kappa} \eta_{\nu\beta} \eta_{\alpha\rho} + 4\eta_{\kappa\lambda} \eta_{\mu\beta} \eta_{\nu\sigma} \eta_{\alpha\rho} \\ &\quad - 4\eta_{\kappa\mu} \eta_{\lambda\beta} \eta_{\nu\sigma} \eta_{\alpha\rho} + 4\eta_{\kappa\beta} \eta_{\mu\lambda} \eta_{\nu\sigma} \eta_{\alpha\rho} - 4\eta_{\sigma\lambda} \eta_{\mu\beta} \eta_{\nu\kappa} \eta_{\alpha\rho} + 4\eta_{\sigma\mu} \eta_{\lambda\beta} \eta_{\nu\kappa} \eta_{\alpha\rho} \\ &\quad - 4\eta_{\sigma\beta} \eta_{\mu\lambda} \eta_{\nu\kappa} \eta_{\alpha\rho} + 4\eta_{\sigma\kappa} \eta_{\mu\beta} \eta_{\nu\lambda} \eta_{\alpha\rho} - 4\eta_{\sigma\mu} \eta_{\kappa\beta} \eta_{\nu\lambda} \eta_{\alpha\rho} + 4\eta_{\sigma\beta} \eta_{\mu\kappa} \eta_{\nu\lambda} \eta_{\alpha\rho} \\ &\quad - 4\eta_{\sigma\kappa} \eta_{\lambda\beta} \eta_{\nu\mu} \eta_{\alpha\rho} + 4\eta_{\sigma\lambda} \eta_{\kappa\beta} \eta_{\nu\mu} \eta_{\alpha\rho} - 4\eta_{\sigma\beta} \eta_{\lambda\kappa} \eta_{\nu\mu} \eta_{\alpha\rho} + 4\eta_{\rho\kappa} \eta_{\lambda\mu} \eta_{\nu\beta} \eta_{\alpha\sigma} \end{aligned}$$

$$\begin{aligned}
& -4\eta_{\rho\lambda}\eta_{\kappa\mu}\eta_{\nu\beta}\eta_{\alpha\sigma} + 4\eta_{\rho\mu}\eta_{\lambda\kappa}\eta_{\nu\beta}\eta_{\alpha\sigma} - 4\eta_{\kappa\lambda}\eta_{\mu\beta}\eta_{\nu\rho}\eta_{\alpha\sigma} + 4\eta_{\kappa\mu}\eta_{\lambda\beta}\eta_{\nu\rho}\eta_{\alpha\sigma} \\
& -4\eta_{\kappa\beta}\eta_{\mu\lambda}\eta_{\nu\rho}\eta_{\alpha\sigma} + 4\eta_{\rho\lambda}\eta_{\mu\beta}\eta_{\nu\kappa}\eta_{\alpha\sigma} - 4\eta_{\rho\mu}\eta_{\lambda\beta}\eta_{\nu\kappa}\eta_{\alpha\sigma} + 4\eta_{\rho\beta}\eta_{\mu\lambda}\eta_{\nu\kappa}\eta_{\alpha\sigma} \\
& -4\eta_{\rho\kappa}\eta_{\mu\beta}\eta_{\nu\lambda}\eta_{\alpha\sigma} + 4\eta_{\rho\mu}\eta_{\kappa\beta}\eta_{\nu\lambda}\eta_{\alpha\sigma} - 4\eta_{\rho\beta}\eta_{\mu\kappa}\eta_{\nu\lambda}\eta_{\alpha\sigma} + 4\eta_{\rho\kappa}\eta_{\lambda\beta}\eta_{\nu\mu}\eta_{\alpha\sigma} \\
& -4\eta_{\rho\lambda}\eta_{\kappa\beta}\eta_{\nu\mu}\eta_{\alpha\sigma} + 4\eta_{\rho\beta}\eta_{\lambda\kappa}\eta_{\nu\mu}\eta_{\alpha\sigma} - 4\eta_{\rho\sigma}\eta_{\lambda\mu}\eta_{\nu\beta}\eta_{\alpha\kappa} + 4\eta_{\rho\lambda}\eta_{\sigma\mu}\eta_{\nu\beta}\eta_{\alpha\kappa} \\
& -4\eta_{\rho\mu}\eta_{\lambda\sigma}\eta_{\nu\beta}\eta_{\alpha\kappa} + 4\eta_{\sigma\lambda}\eta_{\mu\beta}\eta_{\nu\rho}\eta_{\alpha\kappa} - 4\eta_{\sigma\mu}\eta_{\lambda\beta}\eta_{\nu\rho}\eta_{\alpha\kappa} + 4\eta_{\sigma\beta}\eta_{\mu\lambda}\eta_{\nu\rho}\eta_{\alpha\kappa} \\
& -4\eta_{\rho\lambda}\eta_{\mu\beta}\eta_{\nu\sigma}\eta_{\alpha\kappa} + 4\eta_{\rho\mu}\eta_{\lambda\beta}\eta_{\nu\sigma}\eta_{\alpha\kappa} - 4\eta_{\rho\beta}\eta_{\mu\lambda}\eta_{\nu\sigma}\eta_{\alpha\kappa} + 4\eta_{\rho\sigma}\eta_{\mu\beta}\eta_{\nu\lambda}\eta_{\alpha\kappa} \\
& -4\eta_{\rho\mu}\eta_{\sigma\beta}\eta_{\nu\lambda}\eta_{\alpha\kappa} + 4\eta_{\rho\beta}\eta_{\sigma\mu}\eta_{\nu\lambda}\eta_{\alpha\kappa} - 4\eta_{\rho\sigma}\eta_{\lambda\beta}\eta_{\nu\mu}\eta_{\alpha\kappa} + 4\eta_{\rho\lambda}\eta_{\sigma\beta}\eta_{\nu\mu}\eta_{\alpha\kappa} \\
& -4\eta_{\rho\beta}\eta_{\lambda\sigma}\eta_{\nu\mu}\eta_{\alpha\kappa} + 4\eta_{\rho\sigma}\eta_{\kappa\mu}\eta_{\nu\beta}\eta_{\alpha\lambda} - 4\eta_{\rho\kappa}\eta_{\sigma\mu}\eta_{\nu\beta}\eta_{\alpha\lambda} + 4\eta_{\rho\mu}\eta_{\kappa\sigma}\eta_{\nu\beta}\eta_{\alpha\lambda} \\
& -4\eta_{\rho\kappa}\eta_{\mu\beta}\eta_{\nu\rho}\eta_{\alpha\lambda} + 4\eta_{\sigma\mu}\eta_{\kappa\beta}\eta_{\nu\rho}\eta_{\alpha\lambda} - 4\eta_{\sigma\beta}\eta_{\mu\kappa}\eta_{\nu\rho}\eta_{\alpha\lambda} + 4\eta_{\rho\kappa}\eta_{\mu\beta}\eta_{\nu\sigma}\eta_{\alpha\lambda} \\
& -4\eta_{\rho\mu}\eta_{\kappa\beta}\eta_{\nu\sigma}\eta_{\alpha\lambda} + 4\eta_{\rho\beta}\eta_{\mu\kappa}\eta_{\nu\sigma}\eta_{\alpha\lambda} - 4\eta_{\rho\sigma}\eta_{\mu\beta}\eta_{\nu\kappa}\eta_{\alpha\lambda} + 4\eta_{\rho\mu}\eta_{\sigma\beta}\eta_{\nu\kappa}\eta_{\alpha\lambda} \\
& -4\eta_{\rho\beta}\eta_{\mu\sigma}\eta_{\nu\kappa}\eta_{\alpha\lambda} + 4\eta_{\rho\sigma}\eta_{\kappa\beta}\eta_{\nu\mu}\eta_{\alpha\lambda} - 4\eta_{\rho\kappa}\eta_{\sigma\beta}\eta_{\nu\mu}\eta_{\alpha\lambda} + 4\eta_{\rho\beta}\eta_{\kappa\sigma}\eta_{\nu\mu}\eta_{\alpha\lambda} \\
& -4\eta_{\rho\sigma}\eta_{\kappa\lambda}\eta_{\nu\beta}\eta_{\alpha\mu} + 4\eta_{\rho\kappa}\eta_{\sigma\lambda}\eta_{\nu\beta}\eta_{\alpha\mu} - 4\eta_{\rho\lambda}\eta_{\kappa\sigma}\eta_{\nu\beta}\eta_{\alpha\mu} + 4\eta_{\rho\kappa}\eta_{\lambda\beta}\eta_{\nu\rho}\eta_{\alpha\mu} \\
& -4\eta_{\sigma\lambda}\eta_{\kappa\beta}\eta_{\nu\rho}\eta_{\alpha\mu} + 4\eta_{\sigma\beta}\eta_{\lambda\kappa}\eta_{\nu\rho}\eta_{\alpha\mu} - 4\eta_{\rho\kappa}\eta_{\lambda\beta}\eta_{\nu\sigma}\eta_{\alpha\mu} + 4\eta_{\rho\lambda}\eta_{\kappa\beta}\eta_{\nu\sigma}\eta_{\alpha\mu} \\
& -4\eta_{\rho\beta}\eta_{\lambda\kappa}\eta_{\nu\sigma}\eta_{\alpha\mu} + 4\eta_{\rho\sigma}\eta_{\lambda\beta}\eta_{\nu\kappa}\eta_{\alpha\mu} - 4\eta_{\rho\lambda}\eta_{\sigma\beta}\eta_{\nu\kappa}\eta_{\alpha\mu} + 4\eta_{\rho\beta}\eta_{\lambda\sigma}\eta_{\nu\kappa}\eta_{\alpha\mu} \\
& -4\eta_{\rho\sigma}\eta_{\kappa\beta}\eta_{\nu\lambda}\eta_{\alpha\mu} + 4\eta_{\rho\kappa}\eta_{\sigma\beta}\eta_{\nu\lambda}\eta_{\alpha\mu} - 4\eta_{\rho\beta}\eta_{\kappa\sigma}\eta_{\nu\lambda}\eta_{\alpha\mu} + 4\eta_{\rho\sigma}\eta_{\kappa\lambda}\eta_{\mu\beta}\eta_{\alpha\nu} \\
& -4\eta_{\rho\kappa}\eta_{\sigma\lambda}\eta_{\mu\beta}\eta_{\alpha\nu} + 4\eta_{\rho\lambda}\eta_{\kappa\sigma}\eta_{\mu\beta}\eta_{\alpha\nu} - 4\eta_{\sigma\kappa}\eta_{\lambda\beta}\eta_{\mu\rho}\eta_{\alpha\nu} + 4\eta_{\sigma\lambda}\eta_{\kappa\beta}\eta_{\mu\rho}\eta_{\alpha\nu} \\
& -4\eta_{\sigma\beta}\eta_{\lambda\kappa}\eta_{\mu\rho}\eta_{\alpha\nu} + 4\eta_{\rho\kappa}\eta_{\lambda\beta}\eta_{\mu\sigma}\eta_{\alpha\nu} - 4\eta_{\rho\lambda}\eta_{\kappa\beta}\eta_{\mu\sigma}\eta_{\alpha\nu} + 4\eta_{\rho\beta}\eta_{\lambda\kappa}\eta_{\mu\sigma}\eta_{\alpha\nu} \\
& -4\eta_{\rho\sigma}\eta_{\lambda\beta}\eta_{\mu\kappa}\eta_{\alpha\nu} + 4\eta_{\rho\lambda}\eta_{\sigma\beta}\eta_{\mu\kappa}\eta_{\alpha\nu} - 4\eta_{\rho\beta}\eta_{\lambda\sigma}\eta_{\mu\kappa}\eta_{\alpha\nu} + 4\eta_{\rho\sigma}\eta_{\kappa\beta}\eta_{\mu\lambda}\eta_{\alpha\nu} \\
& -4\eta_{\rho\kappa}\eta_{\sigma\beta}\eta_{\mu\lambda}\eta_{\alpha\nu} + 4\eta_{\rho\beta}\eta_{\kappa\sigma}\eta_{\mu\lambda}\eta_{\alpha\nu}. \tag{G.22}
\end{aligned}$$

## Appendix H: Spinor representations of the Lorentz group

The explicit form of the Lagrange density (21.74) for the Dirac field and the appearance of the factor  $\bar{\Psi} = \Psi^\dagger \cdot \gamma^0$  are determined by the requirement of Lorentz invariance of  $\mathcal{L}$  and the transformation properties of spinors under Lorentz transformations. However, before we can elaborate on these points, we have to revisit the Lorentz transformation (B.8), which is also denoted as the vector representation because it acts on spacetime vectors. We can discuss this in general numbers  $n$  of spatial dimensions and  $d = n + 1$  of spacetime dimensions.

### Generators of proper orthochronous Lorentz transformations in the vector and spinor representations

We can write the two factors of a proper orthochronous Lorentz transformation (B.8) as exponentials of Lie algebra elements,

$$\Lambda(\mathbf{u}, \underline{\epsilon}) = \Lambda(\mathbf{u}) \cdot \Lambda(\underline{\epsilon}) = \exp(\mathbf{u} \cdot \mathbf{K}) \cdot \exp\left(\frac{1}{2} \epsilon^{ij} L_{ij}\right). \quad (\text{H.1})$$

For the boost part we use explicit construction to prove that every proper Lorentz boost can be written in the form  $\exp(\mathbf{u} \cdot \mathbf{K})$ .

For the rotation part we can use the general result that every element of a compact Lie group can be written as a single exponential of a corresponding Lie algebra element, or we can use the fact that a general  $n \times n$  rotation matrix consists of  $n$  orthonormal row vectors, which fixes the general form in terms of  $n(n - 1)/2$  parameters, and then demonstrate that the  $n(n - 1)/2$  parameters  $\epsilon^{ij}$  of  $\exp(\epsilon^{ij} L_{ij}/2)$  provide a general parametrization of  $n$  orthonormal row vectors.

Alternatively, we can consider (H.1) as an example for the polar decomposition (F.4) and infer the representation in terms of matrix exponentials from the results on matrix logarithms in Appendix F.

The boost part is

$$\Lambda(\mathbf{u}) = \exp(\mathbf{u} \cdot \mathbf{K}) = \exp(\epsilon^{i0} L_{i0}) = \exp(i\epsilon^{i0} M_{i0}) \quad (\text{H.2})$$

and the spatial rotation is

$$\Lambda(\underline{\epsilon}) = \exp\left(\frac{1}{2}\epsilon^{ij} L_{ij}\right) = \exp\left(\frac{i}{2}\epsilon^{ij} M_{ij}\right), \quad (\text{H.3})$$

where  $\epsilon_{ij}$  is the rotation angle in the  $ij$  plane. The generators are (in the vector representation),

$$(L_{\mu\nu})^\rho{}_\sigma = i(M_{\mu\nu})^\rho{}_\sigma = (\eta^\rho{}_\mu \eta_{\nu\sigma} - \eta^\rho{}_\nu \eta_{\mu\sigma}). \quad (\text{H.4})$$

These matrices generate the Lie algebra  $\mathfrak{so}(1, d-1)$ ,

$$\begin{aligned} [L_{\mu\nu}, L_{\rho\sigma}] &= \eta_{\nu\rho} L_{\mu\sigma} + \eta_{\mu\sigma} L_{\nu\rho} - \eta_{\mu\rho} L_{\nu\sigma} - \eta_{\nu\sigma} L_{\mu\rho} \\ &= -(L_{\mu\nu})_\rho{}^\lambda L_{\lambda\sigma} - (L_{\mu\nu})_\sigma{}^\lambda L_{\rho\lambda}. \end{aligned} \quad (\text{H.5})$$

In 4-dimensional Minkowski space, the angles  $\epsilon_{ij}$  are related to the rotation angles  $\varphi_i$  around the  $x^i$ -axis according to

$$\varphi_i = \frac{1}{2}\epsilon_{ijk}\epsilon_{jk}, \quad \epsilon_{ij} = \epsilon_{ijk}\varphi_k. \quad (\text{H.6})$$

To see how the boost vector  $\mathbf{u}$  is related to the velocity  $\mathbf{v} = c\boldsymbol{\beta}$ , we will explicitly calculate the boost matrix  $\Lambda(\mathbf{u})$ . We have with a contravariant row index and a covariant column index, as in (B.8),

$$\begin{aligned} \mathbf{u} \cdot \mathbf{K} &= u^i L_{i0} = iu^i M_{i0} = \begin{pmatrix} 0 & -u_1 & \dots & -u_{d-1} \\ -u_1 & 0 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -u_{d-1} & 0 & \dots & 0 \end{pmatrix} = \begin{pmatrix} 0 & -\mathbf{u}^T \\ -\mathbf{u} & \underline{0} \end{pmatrix}, \\ (\mathbf{u} \cdot \mathbf{K})^2 &= \begin{pmatrix} \mathbf{u}^2 & \mathbf{0}^T \\ \mathbf{0} & \mathbf{u} \otimes \mathbf{u}^T \end{pmatrix}, \quad (\mathbf{u} \cdot \mathbf{K})^{2n} = u^{2n} \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \hat{\mathbf{u}} \otimes \hat{\mathbf{u}}^T \end{pmatrix}, \end{aligned} \quad (\text{H.7})$$

$$(\mathbf{u} \cdot \mathbf{K})^{2n+1} = u^{2n+1} \begin{pmatrix} 0 & -\hat{\mathbf{u}}^T \\ -\hat{\mathbf{u}} & \underline{0} \end{pmatrix}. \quad (\text{H.8})$$

For the interpretation of the  $(d - 1) \times (d - 1)$  matrices  $\hat{u} \otimes \hat{u}^T$  and  $\underline{1} - \hat{u} \otimes \hat{u}^T$ , note that for every  $(d - 1)$ -dimensional spatial vector  $\mathbf{r}$

$$\mathbf{r}_{\parallel} = \hat{u}(\hat{u}^T \cdot \mathbf{r}) = (\hat{u} \otimes \hat{u}^T) \cdot \mathbf{r}$$

is the part  $\mathbf{r}_{\parallel}$  of the vector which is parallel to  $\mathbf{u}$ , and

$$\mathbf{r}_{\perp} = \mathbf{r} - \mathbf{r}_{\parallel} = (\underline{1} - \hat{u} \otimes \hat{u}^T) \cdot \mathbf{r}$$

is the part of the vector which is orthogonal to  $\mathbf{u}$ .

Substitution of the results (H.7, H.8) into (H.2) yields for the boost in the direction  $\hat{u} = \hat{\beta}$

$$\begin{aligned} \Lambda(\mathbf{u}) &= \begin{pmatrix} \cosh(u) & & \mathbf{0}^T \\ \mathbf{0} & \underline{1} + \hat{u} \otimes \hat{u}^T (\cosh(u) - 1) & \\ & & \end{pmatrix} + \sinh(u) \begin{pmatrix} 0 & -\hat{u}^T \\ -\hat{u} & 0 \end{pmatrix} \\ &= \begin{pmatrix} \gamma & & -\gamma \boldsymbol{\beta}^T \\ -\gamma \boldsymbol{\beta} & \underline{1} - \hat{u} \otimes \hat{u}^T + \gamma \hat{u} \otimes \hat{u}^T & \\ & & \end{pmatrix}, \end{aligned}$$

i.e.

$$\gamma = \cosh(u), \quad \boldsymbol{\beta} = \tanh(u), \quad u = \operatorname{artanh}(\boldsymbol{\beta}) = \frac{1}{2} \ln \left( \frac{1 + \boldsymbol{\beta}}{1 - \boldsymbol{\beta}} \right).$$

The parameter  $u$  is usually denoted as the *boost parameter* or *rapidity* of the Lorentz transformation.

It may also be worthwhile to write down the corresponding rotation matrix in 4-dimensional Minkowski space. If we use the  $3 \times 3$  matrices from Section 7.4 for the spatial subsections of the rotation matrices<sup>1</sup>  $L_{mn}$ ,

$$(L_i)_{jk} = \frac{1}{2} \epsilon_{imn} (L_{mn})_{jk} = \epsilon_{ijk}, \tag{H.9}$$

the rotation matrices take the following form,

$$\Lambda(\underline{\epsilon}) = \exp \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \boldsymbol{\varphi} \cdot \mathbf{L} \end{pmatrix} = \begin{pmatrix} 1 & \mathbf{0}^T \\ \mathbf{0} & \exp(\boldsymbol{\varphi} \cdot \mathbf{L}) \end{pmatrix}, \tag{H.10}$$

with the  $3 \times 3$  rotation matrix

$$\exp(\boldsymbol{\varphi} \cdot \mathbf{L}) = \hat{\boldsymbol{\varphi}} \otimes \hat{\boldsymbol{\varphi}}^T + (\underline{1} - \hat{\boldsymbol{\varphi}} \otimes \hat{\boldsymbol{\varphi}}^T) \cos \varphi + \hat{\boldsymbol{\varphi}} \cdot \mathbf{L} \sin \varphi. \tag{H.11}$$

Application of the matrix  $\hat{\boldsymbol{\varphi}} \cdot \mathbf{L}$  generates a vector product,

$$(\hat{\boldsymbol{\varphi}} \cdot \mathbf{L}) \cdot \mathbf{r} = -\hat{\boldsymbol{\varphi}} \times \mathbf{r}.$$

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<sup>1</sup>In this Appendix we use underscore only for  $2 \times 2$  matrices.

The anticommutation relations (21.35) imply that the properly normalized commutators of  $\gamma$ -matrices,

$$S_{\mu\nu} = \frac{i}{4}[\gamma_\mu, \gamma_\nu] \quad (\text{H.12})$$

also provide a representation of the Lie algebra  $\text{so}(1, d-1)$  (H.5),

$$\begin{aligned} [S_{\mu\nu}, S_{\rho\sigma}] &= i(\eta_{\mu\rho}S_{\nu\sigma} + \eta_{\nu\sigma}S_{\mu\rho} - \eta_{\nu\rho}S_{\mu\sigma} - \eta_{\mu\sigma}S_{\nu\rho}) \\ &= i(L_{\mu\nu})_\rho{}^\lambda S_{\lambda\sigma} + i(L_{\mu\nu})_\sigma{}^\lambda S_{\rho\lambda}. \end{aligned} \quad (\text{H.13})$$

See equations (H.16–H.18) for the proof.

This representation of the Lorentz group is realized in the transformation of Dirac spinors  $\psi(x)$  under Lorentz transformations

$$\begin{aligned} x' &= \Lambda(\epsilon) \cdot x = \exp\left(\frac{1}{2}\epsilon^{\mu\nu}L_{\mu\nu}\right) \cdot x, \\ \psi'(x') &= U(\Lambda) \cdot \psi(x) = \exp\left(\frac{i}{2}\epsilon^{\mu\nu}S_{\mu\nu}\right) \cdot \psi(x). \end{aligned} \quad (\text{H.14})$$

The anticommutation relations (21.35) also imply invariance of the  $\gamma$ -matrices under Lorentz transformations  $x' = \Lambda(\epsilon) \cdot x$ ,

$$\gamma'^\mu = \Lambda^\mu{}_\nu(\epsilon) \exp\left(\frac{i}{2}\epsilon^{\kappa\lambda}S_{\kappa\lambda}\right) \cdot \gamma^\nu \cdot \exp\left(-\frac{i}{2}\epsilon^{\rho\sigma}S_{\rho\sigma}\right) = \gamma^\mu, \quad (\text{H.15})$$

see equation (H.19). This invariance property of the  $\gamma$ -matrices also implies form invariance of the Dirac equation under Lorentz transformations,

$$i\hbar\gamma^\mu\partial'_\mu\psi'(x') - mc\psi'(x') = \exp\left(\frac{i}{2}\epsilon^{\kappa\lambda}S_{\kappa\lambda}\right) \cdot \left(i\hbar\gamma^\mu\partial_\mu\psi(x) - mc\psi(x)\right),$$

*i.e. all inertial observers can use the same set of  $\gamma$ -matrices, and the Dirac equation has the same form for all of them.*

## Verification of the Lorentz commutation relations for the spinor representations

The anti-commutation relations (21.35) imply

$$\begin{aligned} [\gamma_\mu\gamma_\nu, \gamma_\rho] &= \gamma_\mu\{\gamma_\nu, \gamma_\rho\} - \{\gamma_\mu, \gamma_\rho\}\gamma_\nu = 2\eta_{\mu\rho}\gamma_\nu - 2\eta_{\nu\rho}\gamma_\mu \\ &= 2(L_{\mu\nu})_\rho{}^\sigma\gamma_\sigma, \end{aligned} \quad (\text{H.16})$$

where the matrices  $L_{\mu\nu}$  were given in (H.4). Equation (H.16) also implies

$$[S_{\mu\nu}, \gamma_\rho] = i(L_{\mu\nu})_\rho^\sigma \gamma_\sigma \quad (\text{H.17})$$

and

$$\begin{aligned} [S_{\mu\nu}, S_{\rho\sigma}] &= \frac{i}{4} [S_{\mu\nu}, [\gamma_\rho, \gamma_\sigma]] = \frac{i}{4} [[S_{\mu\nu}, \gamma_\rho], \gamma_\sigma] - \frac{i}{4} [[S_{\mu\nu}, \gamma_\sigma], \gamma_\rho] \\ &= -\frac{1}{4} (L_{\mu\nu})_\rho^\lambda [\gamma_\lambda, \gamma_\sigma] + \frac{1}{4} (L_{\mu\nu})_\sigma^\lambda [\gamma_\lambda, \gamma_\rho] \\ &= i(L_{\mu\nu})_\rho^\lambda S_{\lambda\sigma} + i(L_{\mu\nu})_\sigma^\lambda S_{\rho\lambda}. \end{aligned} \quad (\text{H.18})$$

Equation (H.17) implies the Lorentz invariance of the  $\gamma$ -matrices,

$$\begin{aligned} \exp\left(\frac{i}{2}\epsilon^{\mu\nu} S_{\mu\nu}\right) \gamma_\rho \exp\left(-\frac{i}{2}\epsilon^{\kappa\lambda} S_{\kappa\lambda}\right) &= \left[\exp\left(-\frac{1}{2}\epsilon^{\mu\nu} L_{\mu\nu}\right)\right]_\rho^\sigma \gamma_\sigma \\ &= \Lambda^{-1}(\epsilon)_\rho^\sigma \gamma_\sigma. \end{aligned} \quad (\text{H.19})$$

## Scalar products of spinors and the Lagrangian for the Dirac equation

The hermiticity relation (G.10) implies the following hermiticity property of the Lorentz generators,

$$S_{\mu\nu}^+ = \gamma^0 S_{\mu\nu} \gamma^0,$$

and therefore

$$\psi'^+(x') = \psi^+(x) \cdot \gamma^0 \exp\left(-\frac{i}{2}\epsilon^{\mu\nu} S_{\mu\nu}\right) \gamma^0.$$

The adjoint spinor

$$\bar{\psi}(x) = \psi^+(x) \cdot \gamma^0$$

therefore transforms inversely to the spinor  $\psi(x)$ ,

$$\bar{\psi}'(x) = \bar{\psi}(x) \cdot \exp\left(-\frac{i}{2}\epsilon^{\mu\nu} S_{\mu\nu}\right),$$

and the product of spinors

$$\bar{\psi}(x) \cdot \phi(x) = \psi^+(x) \cdot \gamma^0 \cdot \phi(x)$$

is Lorentz invariant. This yields a Lorentz invariant Lagrangian for the Dirac equation,

$$\mathcal{L} = \frac{i\hbar c}{2} \left( \bar{\psi}(x) \cdot \gamma^\mu \cdot \partial_\mu \psi(x) - \partial_\mu \bar{\psi}(x) \cdot \gamma^\mu \cdot \psi(x) \right) - mc^2 \bar{\psi}(x) \cdot \psi(x). \quad (\text{H.20})$$

## The spinor representation in the Weyl and Dirac bases of $\gamma$ -matrices

In *even dimensions*, the construction (G.9) yields  $\gamma$ -matrices of the form

$$\gamma_0 = \begin{pmatrix} 0 & \underline{1} \\ \underline{1} & 0 \end{pmatrix}, \quad \gamma_i = \begin{pmatrix} 0 & \underline{\sigma}_i \\ -\underline{\sigma}_i & 0 \end{pmatrix}, \quad (\text{H.21})$$

with hermitian  $(2^{(d/2)-1} \times 2^{(d/2)-1})$  matrices  $\underline{\sigma}_i$ , which satisfy

$$\{\underline{\sigma}_i, \underline{\sigma}_j\} = 2\delta_{ij}. \quad (\text{H.22})$$

The spinor representation of the Lorentz generators in this Weyl basis is

$$S_{0i} = \frac{i}{2} \gamma_0 \gamma_i = \frac{i}{2} \begin{pmatrix} -\underline{\sigma}_i & 0 \\ 0 & \underline{\sigma}_i \end{pmatrix}, \quad (\text{H.23})$$

$$S_{ij} = \frac{i}{4} [\gamma_i, \gamma_j] = -\frac{i}{4} \begin{pmatrix} [\underline{\sigma}_i, \underline{\sigma}_j] & 0 \\ 0 & [\underline{\sigma}_i, \underline{\sigma}_j] \end{pmatrix}. \quad (\text{H.24})$$

This is the advantage of a Weyl basis: The  $2^{d/2}$  components of a spinor explicitly split into two Weyl spinors with  $2^{(d/2)-1}$  components. The two Weyl spinors transform separately under proper orthochronous Lorentz transformations. A Dirac spinor representation in even dimensions is therefore reducible under the group of proper orthochronous Lorentz transformations. However, the form of  $S_{0i}$  tells us that the two Weyl spinors are transformed into each other under time or space inversions. Therefore the representation of the full Lorentz group really requires the full  $2^{d/2}$ -dimensional Dirac spinor.

The rotation generators in the Dirac representation in even dimensions are the same as in the Weyl basis, but the boost generators become

$$S_{0i} = -\frac{i}{2} \begin{pmatrix} 0 & \underline{\sigma}_i \\ \underline{\sigma}_i & 0 \end{pmatrix}. \quad (\text{H.25})$$

For an *odd number of spacetime dimensions* our construction provides  $\gamma$ -matrices of the form,

$$\gamma_0 = \pm \begin{pmatrix} -\underline{1} & 0 \\ 0 & \underline{1} \end{pmatrix}, \quad \gamma_i = \begin{pmatrix} 0 & \underline{\sigma}_i \\ -\underline{\sigma}_i & 0 \end{pmatrix}, \quad 1 \leq i \leq d-2,$$

$$\gamma_{d-1} = -i \begin{pmatrix} 0 & \underline{1} \\ \underline{1} & 0 \end{pmatrix}.$$

The rotation generators  $S_{ij}$ ,  $1 \leq i, j \leq d-2$ , are the same as in  $d-1$  dimensions, but rotations of the  $(i, d-1)$  plane are generated by

$$S_{i,d-1} = \frac{1}{2} \begin{pmatrix} \underline{\sigma}_i & 0 \\ 0 & -\underline{\sigma}_i \end{pmatrix}, \tag{H.26}$$

and the boost generators are off-diagonal,

$$S_{0i} = \mp \frac{i}{2} \begin{pmatrix} 0 & \underline{\sigma}_i \\ \underline{\sigma}_i & 0 \end{pmatrix}, \quad S_{0,d-1} = \pm \frac{1}{2} \begin{pmatrix} 0 & -\underline{1} \\ \underline{1} & 0 \end{pmatrix}. \tag{H.27}$$

The proper orthochronous Lorentz group therefore mixes all the  $2^{(d-1)/2}$  components of a Dirac spinor in odd dimensions.

### Construction of the vector representation from the spinor representation

Equation (21.35) implies

$$\text{tr}(\gamma_\mu \gamma_\nu) = -2^{\lfloor d/2 \rfloor} \eta_{\mu\nu}. \tag{H.28}$$

This and the invariance of the  $\gamma$ -matrices (H.15) can be used to reconstruct the vector representation of a proper orthochronous Lorentz transformation from the corresponding spinor representation,

$$\Lambda^\mu{}_\nu(\epsilon) = -2^{-\lfloor d/2 \rfloor} \text{tr} \left[ \exp \left( -\frac{i}{2} \epsilon^{\kappa\lambda} S_{\kappa\lambda} \right) \cdot \gamma^\mu \cdot \exp \left( \frac{i}{2} \epsilon^{\rho\sigma} S_{\rho\sigma} \right) \cdot \gamma_\nu \right]. \tag{H.29}$$

We can also use equation (H.28) to transform every vector into a spinor of order 2 (or every tensor of order  $n$  into a spinor of order  $2n$ ),

$$x(\gamma) = x^\mu \gamma_\mu, \quad x^\mu = -2^{-\lfloor d/2 \rfloor} \text{tr}[\gamma^\mu \cdot x(\gamma)],$$

and the invariance of the  $\gamma$ -matrices implies

$$x'^\mu = \Lambda^\mu{}_\nu(\epsilon) x^\nu \Leftrightarrow x'(\gamma) = \exp \left( \frac{i}{2} \epsilon^{\kappa\lambda} S_{\kappa\lambda} \right) \cdot x(\gamma) \cdot \exp \left( -\frac{i}{2} \epsilon^{\rho\sigma} S_{\rho\sigma} \right).$$

## Construction of the free Dirac spinors from Dirac spinors at rest

We use  $c = 1$  and  $d = 4$  in this section. The Dirac equation in momentum space (21.41) is for a Dirac spinor  $\psi(E, \mathbf{0})$  at rest

$$(m - E\gamma^0)\psi(E, \mathbf{0}) = 0. \quad (\text{H.30})$$

The hermitian  $4 \times 4$  matrix  $\gamma^0$  can only have eigenvalues  $\pm 1$ , which each must be two-fold degenerate because  $\gamma^0$  is traceless. Therefore Dirac spinors at rest must correspond to energy eigenvalues  $E = \pm m$ . To construct the free Dirac spinors for arbitrary on-shell momentum 4-vector we can then use a boost into a frame where the fermion has on-shell momentum 4-vector  $\pm p$ ,

$$\begin{pmatrix} \pm E \\ \mathbf{0} \end{pmatrix} \rightarrow \begin{pmatrix} \pm \sqrt{\mathbf{p}^2 + m^2} \\ \pm \mathbf{p} \end{pmatrix} = \Lambda \cdot \begin{pmatrix} \pm m \\ \mathbf{0} \end{pmatrix}, \quad (\text{H.31})$$

and equation (H.14) then implies

$$\psi(\pm \sqrt{\mathbf{p}^2 + m^2}, \pm \mathbf{p}) = U(\Lambda) \cdot \psi(\pm m, \mathbf{0}).$$

The Lorentz boost which takes us from the rest frame of the fermion into a frame where the fermion has on-shell momentum 4-vector  $\pm p$  is

$$\begin{aligned} \Lambda(\mathbf{u}) &= \{\Lambda^\mu{}_\nu(\mathbf{u})\} = \begin{pmatrix} \gamma & & -\gamma\boldsymbol{\beta}^T \\ -\gamma\boldsymbol{\beta} & \mathbf{1} - \hat{\mathbf{u}} \otimes \hat{\mathbf{u}}^T + \gamma\hat{\mathbf{u}} \otimes \hat{\mathbf{u}}^T \end{pmatrix} \\ &= \frac{1}{m} \begin{pmatrix} \sqrt{\mathbf{p}^2 + m^2} & & \mathbf{p}^T \\ \mathbf{p} & m\mathbf{1} - m\hat{\mathbf{p}} \otimes \hat{\mathbf{p}}^T + \sqrt{\mathbf{p}^2 + m^2}\hat{\mathbf{p}} \otimes \hat{\mathbf{p}}^T \end{pmatrix}, \end{aligned}$$

i.e. with  $E(\mathbf{p}) \equiv \sqrt{\mathbf{p}^2 + m^2}$ ,

$$\begin{aligned} \gamma &= \cosh(u) = \frac{1}{m} \sqrt{\mathbf{p}^2 + m^2} = \frac{E(\mathbf{p})}{m}, & \gamma\boldsymbol{\beta} &= \hat{\mathbf{u}} \sinh(u) = -\frac{\mathbf{p}}{m}, \\ \mathbf{v} &= \boldsymbol{\beta} = -\frac{\mathbf{p}}{\sqrt{\mathbf{p}^2 + m^2}}. \end{aligned} \quad (\text{H.32})$$

The minus sign makes perfect sense: We have to transform from the particle's rest frame into a frame which moves with speed  $\mathbf{v} = -\mathbf{v}_{particle}$  relative to the particle to observe the particle with speed  $\mathbf{v}_{particle} = \mathbf{p}/E(\mathbf{p})$ .

The rapidity parameter of the particle is

$$\begin{aligned} u &= \operatorname{artanh}(\beta) = \frac{1}{2} \ln \left( \frac{1 + \beta}{1 - \beta} \right) = \frac{1}{2} \ln \left( \frac{\sqrt{\mathbf{p}^2 + m^2} + |\mathbf{p}|}{\sqrt{\mathbf{p}^2 + m^2} - |\mathbf{p}|} \right) \\ &= \ln \left( \frac{\sqrt{\mathbf{p}^2 + m^2} + |\mathbf{p}|}{m} \right). \end{aligned}$$

The general boost matrix acting on the spinors is

$$\begin{aligned} U(\mathbf{u}) &= \exp(iu^i S_{i0}) = \exp\left(\frac{1}{2}u^i \gamma_0 \gamma_i\right) = \cosh\left(\frac{u}{2}\right) + \hat{\mathbf{u}} \cdot \gamma_0 \boldsymbol{\gamma} \sinh\left(\frac{u}{2}\right), \\ U^2(\mathbf{u}) &= \exp(2iu^i S_{i0}) = \exp(u^i \gamma_0 \gamma_i) = \cosh(u) + \hat{\mathbf{u}} \cdot \gamma_0 \boldsymbol{\gamma} \sinh(u). \end{aligned}$$

In the present case we have

$$U^2(\mathbf{u}) = \frac{1}{m} \left( \sqrt{\mathbf{p}^2 + m^2} - \mathbf{p} \cdot \gamma_0 \boldsymbol{\gamma} \right),$$

i.e. we can also write

$$U(\mathbf{u}) = \frac{1}{\sqrt{m}} \sqrt{\sqrt{\mathbf{p}^2 + m^2} - \mathbf{p} \cdot \gamma_0 \boldsymbol{\gamma}}. \quad (\text{H.33})$$

The corresponding boost matrices in the Dirac representation (21.36) are

$$\begin{aligned} \gamma_0 \gamma_i &= \begin{pmatrix} 0 & -\underline{\sigma}_i \\ -\underline{\sigma}_i & 0 \end{pmatrix}, \\ U(\mathbf{u}) &= \begin{pmatrix} \cosh\left(\frac{u}{2}\right) & -\hat{\mathbf{u}}^T \cdot \underline{\boldsymbol{\sigma}} \sinh\left(\frac{u}{2}\right) \\ -\hat{\mathbf{u}} \cdot \underline{\boldsymbol{\sigma}} \sinh\left(\frac{u}{2}\right) & \cosh\left(\frac{u}{2}\right) \end{pmatrix} = \frac{1}{\sqrt{m}} \begin{pmatrix} E(\mathbf{p}) & \mathbf{p} \cdot \underline{\boldsymbol{\sigma}} \\ \mathbf{p} \cdot \underline{\boldsymbol{\sigma}} & E(\mathbf{p}) \end{pmatrix}^{1/2}. \end{aligned}$$

For the evaluation of the hyperbolic functions, we note

$$\begin{aligned} \cosh\left(\frac{u}{2}\right) &= \sqrt{\frac{\cosh(u) + 1}{2}} = \sqrt{\frac{E(\mathbf{p}) + m}{2m}}, \\ \sinh\left(\frac{u}{2}\right) &= \sqrt{\frac{\cosh(u) - 1}{2}} = \sqrt{\frac{E(\mathbf{p}) - m}{2m}} = \frac{|\mathbf{p}|}{\sqrt{2m(E(\mathbf{p}) + m)}}. \end{aligned}$$

This yields

$$U(\mathbf{u}) = \frac{1}{\sqrt{2m(E(\mathbf{p}) + m)}} \begin{pmatrix} E(\mathbf{p}) + m & \mathbf{p} \cdot \underline{\boldsymbol{\sigma}} \\ \mathbf{p} \cdot \underline{\boldsymbol{\sigma}} & E(\mathbf{p}) + m \end{pmatrix}. \quad (\text{H.34})$$

The rest frame spinors satisfying equation (H.30) in the Dirac representation are

$$u(\mathbf{0}, \frac{1}{2}) = \begin{pmatrix} \sqrt{2m} \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad u(\mathbf{0}, -\frac{1}{2}) = \begin{pmatrix} 0 \\ \sqrt{2m} \\ 0 \\ 0 \end{pmatrix},$$

$$v(\mathbf{0}, -\frac{1}{2}) = \begin{pmatrix} 0 \\ 0 \\ \sqrt{2m} \\ 0 \end{pmatrix}, \quad v(\mathbf{0}, \frac{1}{2}) = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \sqrt{2m} \end{pmatrix},$$

and application of the spinor boost matrix (H.34) yields the spinors  $u(\mathbf{p}, \pm\frac{1}{2})$  and  $v(\mathbf{p}, \pm\frac{1}{2})$  in agreement with equations (21.45–21.48). The initial construction there from  $m - \gamma \cdot p$  gave us the negative energy solutions  $v(-\mathbf{p}, \pm\frac{1}{2})$  for momentum 4-vector  $(-E(\mathbf{p}), \mathbf{p})$ , whereas the construction from equation (H.31) gave us directly the negative energy solutions  $v(\mathbf{p}, \pm\frac{1}{2})$  for momentum 4-vector  $-p = (-E(\mathbf{p}), -\mathbf{p})$ , which in either derivation are finally used in the general free solution (21.49).

# Appendix I: Transformation of fields under reflections

In this Appendix we will assume  $d = 4$  for the number of spacetime dimensions. The proper orthochronous Lorentz transformations were introduced in Appendix B and we have discussed exponential representations of boosts and rotations in equations (H.1–H.27). However, the relativistic line element  $ds^2 = -\eta_{\mu\nu}dx^\mu dx^\nu$  is also invariant under reflections<sup>1</sup>

$$P_\mu : dx^\mu \rightarrow -dx^\mu, \quad dx^\nu \rightarrow dx^\nu \ (v \neq \mu).$$

The product of any two spatial reflections is a rotation of the corresponding spatial plane by  $\pi$ , cf. (H.10, H.11),

$$P_i P_j = \exp(i\pi M_{ij}),$$

and this implies that we can write any particular spatial reflection as a combination of the reflection  $P = P_1 P_2 P_3$  of all spatial directions with a rotation by  $\pi$ ,

$$P_i = P \exp\left(\frac{i}{2} \pi \epsilon_{ijk} M_{jk}\right).$$

Therefore it is sufficient to discuss the two discrete Lorentz transformations  $T = P_0$  (reversal of time direction) and  $P$ . The spatial inversion  $P$  is also denoted as a *parity transformation*.

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<sup>1</sup>The reflections  $dt \rightarrow -dt$  or  $dx^i \rightarrow -dx^i$  (or up to constant shifts,  $t \rightarrow -t$ ,  $x^i \rightarrow -x^i$ ) are usually denoted as time or space *inversions*. This convention likely originated from the fact that in algebraic fields (here “field” refers to the mathematical definition of a set which allows for addition, subtraction, multiplication, and division where possible)  $x \rightarrow -x$  is the inversion operation with respect to addition. However, the operations  $P_\mu$  are reversals of time or spatial directions which arise from reflections at 3-dimensional hyperplanes located at some coordinate value  $X^\mu$ :  $x^\mu \rightarrow 2X^\mu - x^\mu$ . Therefore we prefer the designation *reflections* for these transformations.

We can determine the transformation properties of fields under P and T from the requirement that electrodynamics should be invariant under these transformations, i.e. we postulate that the equations

$$[\hbar\partial - iQA]^2\phi - m^2c^2\phi = 0, \quad \gamma^\mu[i\hbar\partial_\mu + qA_\mu]\Psi - mc\Psi = 0, \quad (\text{I.1})$$

$$-\frac{1}{\mu_0c}\partial_\mu F^{\mu\nu} = q\bar{\Psi}\gamma^\nu\Psi + iQc\left[\partial^\nu\phi^+ \cdot \phi - \phi^+ \cdot \partial^\nu\phi + i\frac{Q}{\hbar}\phi^+A^\nu\phi\right] \quad (\text{I.2})$$

hold in this form also for an observer that uses reflected spatial axes or uses decreasing values of  $t$  to label the future.

We know already from classical electrodynamics how electromagnetic fields and charge distributions transform under P and T, see e.g. [19],

$$\text{T: } t' = -t, \quad \mathbf{x}' = \mathbf{x}, \quad j'_0(\mathbf{x}, t) = j_0(\mathbf{x}, -t), \quad \mathbf{j}'(\mathbf{x}, t) = -\mathbf{j}(\mathbf{x}, -t),$$

$$\mathbf{E}'(\mathbf{x}, t) = \mathbf{E}(\mathbf{x}, -t), \quad \mathbf{B}'(\mathbf{x}, t) = -\mathbf{B}(\mathbf{x}, -t),$$

$$\text{P: } t' = t, \quad \mathbf{x}' = -\mathbf{x}, \quad j'_0(\mathbf{x}, t) = j_0(-\mathbf{x}, t), \quad \mathbf{j}'(\mathbf{x}, t) = -\mathbf{j}(-\mathbf{x}, t),$$

$$\mathbf{E}'(\mathbf{x}, t) = -\mathbf{E}(-\mathbf{x}, t), \quad \mathbf{B}'(\mathbf{x}, t) = \mathbf{B}(-\mathbf{x}, t).$$

The transformation properties of the electromagnetic fields imply that (up to gauge transformations) the vector potentials transform according to

$$\text{T: } A'_0(\mathbf{x}, t) = A_0(\mathbf{x}, -t), \quad \mathbf{A}'(\mathbf{x}, t) = -\mathbf{A}(\mathbf{x}, -t),$$

$$\text{P: } A'_0(\mathbf{x}, t) = A_0(-\mathbf{x}, t), \quad \mathbf{A}'(\mathbf{x}, t) = -\mathbf{A}(-\mathbf{x}, t).$$

The components of  $A_\mu(x)$  transform under P like the derivative operators  $\partial_\mu$ , such that the covariant derivatives transform like  $D'_0 = D_0$ ,  $D'_i = -D_i$ . We can therefore get the correct transformation behavior of the currents on the right hand side of Maxwell's equations (I.2) and preserve the matter equations (I.1) if we transform the matter fields (up to gauge transformations) according to

$$\text{P: } \phi'(\mathbf{x}, t) = \phi(-\mathbf{x}, t), \quad \Psi'(\mathbf{x}, t) = \gamma^0\Psi(-\mathbf{x}, t).$$

On the other hand, the partial derivatives and vector potentials pick up relative minus signs under time reversal T:

$$\hbar\partial_0 - iqA_0(\mathbf{x}, t) = -\hbar\partial'_0 - iqA'_0(\mathbf{x}, t'), \quad \hbar\nabla - iq\mathbf{A}(\mathbf{x}, t) = \hbar\nabla + iq\mathbf{A}(\mathbf{x}, t').$$

The transformation properties of scalar and spinor fields under time reversal therefore need to invoke complex conjugations to preserve the matter equations of motion (I.1), and they need to reverse the signs of some of the derivatives of the Dirac field after complex conjugation while leaving the other derivative terms

unchanged. In a Dirac or Weyl basis of  $\gamma$  matrices (21.36, 21.37), this can be achieved (up to gauge transformations) through the transformation laws<sup>2</sup>

$$T : \phi'(\mathbf{x}, t) = \phi^*(\mathbf{x}, -t), \quad \Psi'(\mathbf{x}, t) = \gamma_1 \gamma_3 \Psi^*(\mathbf{x}, -t).$$

Relativistic electrodynamics is invariant under P and T and also under charge conjugation (21.3, 21.79). However, as a general property relativistic field theories only need to be invariant under the combination CPT, see e.g. Vol. I of [41], which also provides original references for the CPT theorem. In our conventions, CPT acts on scalar and spinor fields and real vector potentials according to

$$\text{CPT} : \phi'(x) = \phi(-x), \quad \Psi'(x) = \gamma_5 \Psi(-x), \quad A'_\mu(x) = A_\mu(-x).$$

Here the  $\gamma_5$  matrix is defined as

$$\gamma_5 = i\gamma^0 \gamma^1 \gamma^2 \gamma^3.$$

It takes the following explicit forms in the Dirac or Weyl representations:

$$\gamma_5^{(D)} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma_5^{(W)} = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

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<sup>2</sup>Time reversal and charge conjugation also require a transposition of operator products if the fermionic field  $\Psi$  is not a  $c$  number field but an operator.

## Appendix J: Green's functions in $d$ dimensions

We denote the number of spatial dimensions with  $d$  in this appendix, and we *suspend* the use of summation convention until we reach (J.62).

Green's functions are solutions of linear differential equations with  $\delta$  function source terms. Basic one-dimensional examples are provided by the conditions

$$\frac{d}{dx}S(x) - \kappa S(x) = -\delta(x), \quad \frac{d^2}{dx^2}G(x) - \kappa^2 G(x) = -\delta(x), \quad (\text{J.1})$$

with solutions

$$G(x) = \frac{a}{2\kappa} \exp(-\kappa|x|) + \frac{a-1}{2\kappa} \exp(\kappa|x|) + A \exp(\kappa x) + B \exp(-\kappa x), \quad (\text{J.2})$$

and

$$\begin{aligned} S(x) &= \frac{d}{dx}G(x) + \kappa G(x) \\ &= a\Theta(-x) \exp(\kappa x) + (a-1)\Theta(x) \exp(\kappa x) + 2\kappa A \exp(\kappa x) \\ &= C \exp(\kappa x) + \Theta(-x) \exp(\kappa x) = C' \exp(\kappa x) - \Theta(x) \exp(\kappa x), \quad (\text{J.3}) \\ C' &= C + 1 = 2\kappa A + a. \end{aligned}$$

That the functions (J.2, J.3) satisfy the conditions (J.1) is easily confirmed by using

$$\frac{d}{dx}|x| = \Theta(x) - \Theta(-x), \quad \frac{d}{dx}\Theta(\pm x) = \pm\delta(x).$$

The solutions of the conditions in the limit  $\kappa \rightarrow 0$  are

$$G(x) = \alpha x + \beta - \frac{|x|}{2}, \quad S(x) = \frac{d}{dx}G(x) = \alpha + \frac{\Theta(-x) - \Theta(x)}{2}. \quad (\text{J.4})$$

The appearance of integration constants signals that we can impose boundary conditions on the Green's functions. An important example for this is the requirement of vanishing Green's functions at spatial infinity, which can be imposed if the real part of  $\kappa$  does not vanish. For positive real  $\kappa$  this implies the one-dimensional Green's functions

$$G(x) = \frac{1}{2\kappa} \exp(-\kappa|x|), \quad S(x) = \Theta(-x) \exp(\kappa x).$$

However, in one dimension we cannot satisfy the boundary condition of vanishing Green's functions at infinity if  $\kappa = 0$ , and we will find the same result for the scalar Green's function  $G(\mathbf{x})$  in two dimensions. We can satisfy conditions that the Green's functions (J.4) should vanish on a half-axis  $x < 0$  or  $x > 0$  for  $\kappa = 0$  by choosing  $\alpha = \mp 1/2$ ,  $\beta = 0$ . On the other hand, if  $\kappa = ik$  is imaginary with  $k > 0$ , the Green's function

$$G(x) = \frac{i}{2k} \exp(ik|x|)$$

describes the spatial factor of outgoing waves  $\exp[i(k|x| - \omega t)]$ , i.e. the one-dimensional version of outgoing spherical waves.

## Green's functions for Schrödinger's equation

We are mostly concerned with Green's functions associated with time-independent Hamilton operators

$$H = \frac{\mathbf{p}^2}{2m} + V(\mathbf{x}) = \int d^d \mathbf{x} |\mathbf{x}\rangle \left( -\frac{\hbar^2}{2m} \Delta + V(\mathbf{x}) \right) \langle \mathbf{x}|.$$

Note that the number of spatial dimensions  $d$  is left as a discrete variable.

The inversion condition for the energy-dependent Schrödinger operator,

$$(E - H) \mathcal{G}_{d,V}(E) = 1 \tag{J.5}$$

is in  $\mathbf{x}$  representation the condition

$$\left( E + \frac{\hbar^2}{2m} \Delta - V(\mathbf{x}) \right) \langle \mathbf{x} | \mathcal{G}_{d,V}(E) | \mathbf{x}' \rangle = \delta(\mathbf{x} - \mathbf{x}'). \tag{J.6}$$

The equations (J.5) and (J.6) show that we should rather talk about a Green's operator  $\mathcal{G}_{d,V}(E)$  (or a *resolvent* in mathematical terms), with matrix elements  $\langle \mathbf{x} | \mathcal{G}_{d,V}(E) | \mathbf{x}' \rangle$ . We will instead continue to use the designation Green's function both for  $\mathcal{G}_{d,V}(E)$  and the Fourier transformed operator  $\mathcal{G}_{d,V}(t)$  and for all their

representations in  $\mathbf{x}$  or  $\mathbf{k}$  space variables (or their matrix elements with respect to any other quantum states). The designation Green's function originated from the matrix elements  $\mathcal{G}_{d,V}(\mathbf{x}, \mathbf{x}'; E) \equiv \langle \mathbf{x} | \mathcal{G}_{d,V}(E) | \mathbf{x}' \rangle$ . These functions preceded the resolvent  $\mathcal{G}_{d,V}(E)$  because the inception of differential equations preceded the discovery of abstract operator concepts and bra-ket notation.

The Green's function  $\mathcal{G}_{d,V}(E)$  can eventually be calculated perturbatively in terms of the free Green's function  $\mathcal{G}_d(E) \equiv \mathcal{G}_{d,V=0}(E)$ . The equations

$$(E - H_0) \mathcal{G}_{d,V}(E) = 1 + V \mathcal{G}_{d,V}(E), \quad (E - H_0) \mathcal{G}_d(E) = 1, \quad (\text{J.7})$$

yield

$$\begin{aligned} \mathcal{G}_{d,V}(E) &= \mathcal{G}_d(E) + \mathcal{G}_d(E) V \mathcal{G}_{d,V}(E) \\ &= \mathcal{G}_d(E) + \mathcal{G}_d(E) V \mathcal{G}_d(E) + \mathcal{G}_d(E) V \mathcal{G}_d(E) V \mathcal{G}_{d,V}(E) \\ &= \sum_{n=0}^{\infty} \mathcal{G}_d(E) (V \mathcal{G}_d(E))^n = \sum_{n=0}^{\infty} (\mathcal{G}_d(E) V)^n \mathcal{G}_d(E). \end{aligned} \quad (\text{J.8})$$

From the geometric series appearing in (J.8) we can also find the representations

$$\mathcal{G}_{d,V}(E) = \mathcal{G}_d(E) \frac{1}{1 - V \mathcal{G}_d(E)} = \frac{1}{1 - \mathcal{G}_d(E) V} \mathcal{G}_d(E)$$

which are of course equivalent to the original condition  $(E - H) \mathcal{G}_{d,V}(E) = 1$  through

$$\begin{aligned} (E - H_0 - V)^{-1} &= \left( (E - H_0) \left[ 1 - (E - H_0)^{-1} V \right] \right)^{-1} \\ &= \left( 1 - (E - H_0)^{-1} V \right)^{-1} (E - H_0)^{-1} \end{aligned}$$

and the corresponding relation with  $E - H_0$  extracted on the right hand side of  $V$ .

Whether the formal iteration (J.8) yields a sensible numerical approximation depends on the potential  $V$ , the energy  $E$ , and on the states for which we wish to calculate the corresponding matrix element of  $\mathcal{G}_{d,V}(E)$ . We defined  $H_0 = \mathbf{p}^2/2m$  as the free Hamiltonian, and we have used the first two terms of (J.8) in potential scattering theory in the Born approximation. Other applications of series like (J.8) in perturbation theory would include a solvable part  $V_0$  of the potential in  $H_0$  and use only a perturbation  $V' = V - V_0$  for the iterative solution. However, our main concern in the following will be the free Green's function  $\mathcal{G}_d(E)$ .

The variable  $E$  in (J.5) can be complex, but  $\mathcal{G}_{d,V}(E)$  will become singular for values of  $E$  in the spectrum of  $H$ . It is therefore useful to explicitly add a small imaginary part if  $E$  is constrained to be real, which is the most relevant case for us. To discuss the implications of a small imaginary addition to  $E$ , consider Fourier transformation of (J.5) into the time domain. Substitution of

$$\mathcal{G}_{d,v}(E) = \int_{-\infty}^{\infty} dt \mathcal{G}_{d,v}(t) \exp(iEt/\hbar), \quad (\text{J.9})$$

$$\mathcal{G}_{d,v}(t) = \frac{1}{2\pi\hbar} \int_{-\infty}^{\infty} dE \mathcal{G}_{d,v}(E) \exp(-iEt/\hbar), \quad (\text{J.10})$$

yields

$$\left( i\hbar \frac{d}{dt} - H \right) \mathcal{G}_{d,v}(t) = \delta(t). \quad (\text{J.11})$$

We can solve this equation in the form

$$\mathcal{G}_{d,v}(t) = \frac{a}{i\hbar} \Theta(t) \mathcal{K}_{d,v}(t) + \frac{a-1}{i\hbar} \Theta(-t) \mathcal{K}_{d,v}(t) = \frac{a - \Theta(-t)}{i\hbar} \mathcal{K}_{d,v}(t), \quad (\text{J.12})$$

if  $\mathcal{K}_{d,v}(t)$  is the solution of the time-dependent Schrödinger equation

$$\left( i\hbar \frac{d}{dt} - H \right) \mathcal{K}_{d,v}(t) = 0$$

with initial condition  $\mathcal{K}_{d,v}(0) = 1$ . Indeed, we have found this solution and used it extensively in Chapter 13. It is the time evolution operator

$$\mathcal{K}_{d,v}(t) = U(t) = \exp\left(-\frac{i}{\hbar} Ht\right). \quad (\text{J.13})$$

Equations (J.12) and (J.13) imply that the Green's function in the energy representation is

$$\begin{aligned} \mathcal{G}_{d,v}(E) &= \frac{a}{i\hbar} \int_0^{\infty} dt \exp[i(E - H + i\epsilon)t/\hbar] \\ &\quad - \frac{1-a}{i\hbar} \int_{-\infty}^0 dt \exp[i(E - H - i\epsilon)t/\hbar] \\ &= \frac{a}{E - H + i\epsilon} + \frac{1-a}{E - H - i\epsilon}, \end{aligned} \quad (\text{J.14})$$

with a small shift  $\epsilon > 0$ .

The time-dependent Green's function (J.12) solves the inhomogeneous equation

$$\left( i\hbar \frac{d}{dt} - H \right) F(t) = J(t)$$

in the form

$$\begin{aligned}
 F(t) &= F_0(t) + \int_{-\infty}^{\infty} dt' \mathcal{G}_{d,v}(t-t')J(t') \\
 &= F_0(t) + \frac{a}{i\hbar} \int_{-\infty}^t dt' \exp\left(-\frac{i}{\hbar}H(t-t')\right) J(t') \\
 &\quad + \frac{a-1}{i\hbar} \int_t^{\infty} dt' \exp\left(-\frac{i}{\hbar}H(t-t')\right) J(t'), \tag{J.15}
 \end{aligned}$$

where  $F_0(t)$  is an arbitrary solution of the Schrödinger equation

$$\left(i\hbar \frac{d}{dt} - H\right) F_0(t) = 0.$$

The Green's function (J.12, J.14) with  $a = 1$  is the *retarded Green's function*, because the solution (J.15) receives only contributions from  $J(t')$  at times  $t' < t$  for  $a = 1$ . The Green's function with  $a = 0$  is denoted as an *advanced Green's function*, because it determines  $F(t)$  from back evolution of future values of  $J(t)$ .

We will now specialize to the retarded free Green's function. So far we have found the following representations for this Green's function,

$$\mathcal{G}_d(t) = \frac{\Theta(t)}{i\hbar} \exp\left(-\frac{it}{2m\hbar} \mathbf{p}^2\right), \tag{J.16}$$

$$\mathcal{G}_d(E) = -\frac{2m}{\hbar^2} G_d(E) = \frac{1}{E + i\epsilon - (\mathbf{p}^2/2m)}. \tag{J.17}$$

The rescaled Green's function  $G_d(E)$  is an inverse Poincaré operator

$$\left(\Delta + \frac{2mE}{\hbar^2}\right) \langle \mathbf{x} | G_d(E) | \mathbf{x}' \rangle = -\delta(\mathbf{x} - \mathbf{x}'), \tag{J.18}$$

and has been introduced to make the connection with electromagnetic Green's functions and potentials more visible.

The equations (J.16, J.17) do not generate any spectacular dependence on the number  $d$  of spatial dimensions in the  $\mathbf{k}$ -space representation of the retarded free Green's functions,

$$\begin{aligned}
 \langle \mathbf{k} | \mathcal{G}_d(t) | \mathbf{k}' \rangle &= \frac{\Theta(t)}{i\hbar} \exp\left(-i\frac{\hbar t}{2m} \mathbf{k}^2\right) \delta(\mathbf{k} - \mathbf{k}') \equiv \mathcal{G}_d(\mathbf{k}, t) \delta(\mathbf{k} - \mathbf{k}'), \\
 \langle \mathbf{k} | G_d(E) | \mathbf{k}' \rangle &= \frac{\delta(\mathbf{k} - \mathbf{k}')}{\mathbf{k}^2 - (2mE/\hbar^2) - i\epsilon} \equiv G_d(\mathbf{k}, E) \delta(\mathbf{k} - \mathbf{k}'), \tag{J.19}
 \end{aligned}$$

and also the  $d$ -dependence of the mixed representations is not particularly noteworthy, e.g.

$$\begin{aligned}\langle \mathbf{x} | \mathcal{G}_d(t) | \mathbf{k} \rangle &= \langle \mathbf{x} | \mathbf{k} \rangle \mathcal{G}_d(\mathbf{k}, t) = \frac{\Theta(t)}{i\hbar \sqrt{2\pi}^d} \exp\left(i\mathbf{k} \cdot \mathbf{x} - i \frac{\hbar t}{2m} \mathbf{k}^2\right), \\ \langle \mathbf{x} | G_d(E) | \mathbf{k} \rangle &= \langle \mathbf{x} | \mathbf{k} \rangle G_d(\mathbf{k}, E) = \frac{1}{\sqrt{2\pi}^d} \frac{\exp(i\mathbf{k} \cdot \mathbf{x})}{\mathbf{k}^2 - (2mE/\hbar^2) - i\epsilon}.\end{aligned}$$

The  $\mathbf{x}$ -representation of the time-dependent Green's function,

$$\langle \mathbf{x} | \mathcal{G}_d(t) | \mathbf{x}' \rangle = \frac{1}{(2\pi)^d} \int d^d \mathbf{k} \mathcal{G}_d(\mathbf{k}, t) \exp[i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')] \equiv \mathcal{G}_d(\mathbf{x} - \mathbf{x}', t),$$

is

$$\begin{aligned}\mathcal{G}_d(\mathbf{x}, t) &= \frac{\Theta(t)}{i\hbar (2\pi)^d} \int d^d \mathbf{k} \exp\left[i\left(\mathbf{k} \cdot \mathbf{x} - \frac{\hbar t}{2m} \mathbf{k}^2\right)\right] \\ &= \frac{\Theta(t)}{i\hbar} \sqrt{\frac{m^{-d}}{2\pi i\hbar t}} \exp\left(i \frac{m\mathbf{x}^2}{2\hbar t}\right).\end{aligned}\tag{J.20}$$

This equation holds in the sense that  $\mathcal{G}_d(\mathbf{x} - \mathbf{x}', t - t')$  has to be integrated with an absolutely or square integrable function  $J(\mathbf{x}', t')$  to yield a solution  $F(\mathbf{x}, t)$  (J.15) of an inhomogeneous Schrödinger equation.

The representation of the retarded free Green's function in the time-domain is interesting in its own right, but in terms of dependence on the number  $d$  of dimensions, the operator  $i\hbar \mathcal{G}_d(t)$  and its representations  $i\hbar \mathcal{G}_d(\mathbf{k}, t)$  and  $i\hbar \mathcal{G}_d(\mathbf{x}, t)$  are simply products of  $d$  copies of the corresponding one-dimensional Green's function  $i\hbar \mathcal{G}_1(t)$  and its representations. Free propagation in time separates completely in spatial dimensions<sup>1</sup>.

The interesting dimensional aspects of the Green's function appear if we represent it in the energy domain and in  $\mathbf{x}$ -space,

$$\begin{aligned}\langle \mathbf{x} | G_d(E) | \mathbf{x}' \rangle &= \frac{1}{(2\pi)^d} \int d^d \mathbf{k} G_d(\mathbf{k}, E) \exp[i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')] \\ &\equiv G_d(\mathbf{x} - \mathbf{x}', E).\end{aligned}\tag{J.21}$$

This requires a little extra preparation.

<sup>1</sup>This is a consequence of the separation of the free non-relativistic Hamiltonian  $H_0 = \mathbf{p}^2/2m$ . However, this property does not hold in relativistic quantum mechanics, and therefore the free time-dependent Green's function in the relativistic case is not a product of one-dimensional Green's functions, see (J.44).

### Polar coordinates in $d$ dimensions

Evaluation of the  $d$ -dimensional Fourier transformation in (J.21) involves polar coordinates in  $d$ -dimensional  $\mathbf{k}$  space. Furthermore, it is also instructive to derive the zero energy Green's function  $G_d(0)$  directly in  $\mathbf{x}$  space, which is also conveniently done in polar coordinates. Therefore we use  $\mathbf{x}$  space as a paradigm for the discussion of polar coordinates in  $d$  dimensions with the understanding that in  $\mathbf{k}$  space,  $r = \sqrt{\mathbf{x}^2}$  is replaced with  $k = \sqrt{\mathbf{k}^2}$ .

We define polar coordinates  $r, \theta_1, \dots, \theta_{d-1}$  in  $d$  dimensions through

$$\begin{aligned} x_1 &= r \sin \theta_1 \cdot \sin \theta_2 \cdot \dots \cdot \sin \theta_{d-2} \cdot \sin \theta_{d-1}, & \varphi &= \frac{\pi}{2} - \theta_{d-1} \\ x_2 &= r \sin \theta_1 \cdot \sin \theta_2 \cdot \dots \cdot \sin \theta_{d-2} \cdot \cos \theta_{d-1}, \\ &\vdots \\ x_{d-1} &= r \sin \theta_1 \cdot \cos \theta_2, \\ x_d &= r \cos \theta_1. \end{aligned}$$

This yields corresponding tangent vectors along the radial coordinate lines, cf. (5.18),

$$\mathbf{a}_r = \frac{\partial \mathbf{x}}{\partial r} = \mathbf{e}_r,$$

and along the  $\theta_i$  coordinate lines

$$\mathbf{a}_i = \frac{\partial \mathbf{x}}{\partial \theta_i} = r \sin \theta_1 \cdot \sin \theta_2 \cdot \dots \sin \theta_{i-1} \mathbf{e}_i.$$

Here we defined the unit tangent vector along the  $\theta_i$  coordinate line

$$\mathbf{e}_i = \frac{\mathbf{a}_i}{|\mathbf{a}_i|}.$$

This should not be confused with Cartesian basis vectors since we do not use any Cartesian basis vector in this section.

The induced metric is  $g_{\mu\nu} = \mathbf{a}_\mu \cdot \mathbf{a}_\nu$ , see Section 5.4. This yields in the present case

$$g_{\mu\nu} \Big|_{\mu \neq \nu} = 0, \quad g_{rr} = 1,$$

and

$$g_{ii} = r^2 \sin^2 \theta_1 \cdot \sin^2 \theta_2 \cdot \dots \cdot \sin^2 \theta_{i-1}, \quad 1 \leq i \leq d - 1.$$

The Jacobian determinant (5.28) of the transformation from polar to Cartesian coordinates and the related volume measure (5.27) are then

$$\sqrt{g} = r^{d-1} \sin^{d-2} \theta_1 \cdot \sin^{d-3} \theta_2 \cdot \dots \cdot \sin \theta_{d-2}$$

and

$$d^d \mathbf{x} = dr d\theta_1 \dots d\theta_{d-1} r^{d-1} \sin^{d-2} \theta_1 \cdot \sin^{d-3} \theta_2 \cdot \dots \cdot \sin \theta_{d-2}. \quad (\text{J.22})$$

In particular, the hypersurface area of the  $(d-1)$ -dimensional unit sphere is

$$S_{d-1} = 2\pi \prod_{n=1}^{d-2} \int_0^\pi d\theta \sin^n \theta = \frac{2\sqrt{\pi}^d}{\Gamma(d/2)}. \quad (\text{J.23})$$

The gradient operator  $\nabla = \sum_\mu \mathbf{a}^\mu \partial_\mu$  is

$$\nabla = \mathbf{e}_r \frac{\partial}{\partial r} + \sum_{i=1}^{d-1} \frac{\mathbf{e}_i}{r \sin \theta_1 \cdot \sin \theta_2 \cdot \dots \cdot \sin \theta_{i-1}} \frac{\partial}{\partial \theta_i}.$$

For the calculation of the Laplace operator, we need the derivatives (recall that we do not use summation convention in this appendix)

$$\mathbf{e}_j \cdot \frac{\partial \mathbf{e}_r}{\partial \theta_j} = \sin \theta_1 \cdot \sin \theta_2 \cdot \dots \cdot \sin \theta_{j-1}$$

and

$$\mathbf{e}_j \cdot \frac{\partial \mathbf{e}_i}{\partial \theta_j} = \delta_{j,i+1} \cos \theta_i + \Theta(j > i + 1) \cos \theta_i \cdot \sin \theta_{i+1} \cdot \dots \cdot \sin \theta_{j-1}.$$

This yields

$$\begin{aligned} \Delta &= \frac{\partial^2}{\partial r^2} + \frac{d-1}{r} \frac{\partial}{\partial r} + \frac{1}{r^2} \sum_{i=1}^{d-1} \frac{1}{\sin^2 \theta_1 \cdot \sin^2 \theta_2 \cdot \dots \cdot \sin^2 \theta_{i-1}} \frac{\partial^2}{\partial \theta_i^2} \\ &+ \frac{1}{r^2} \sum_{i=1}^{d-2} \sum_{j=i+1}^{d-1} \frac{\cot \theta_i}{\sin^2 \theta_1 \cdot \sin^2 \theta_2 \cdot \dots \cdot \sin^2 \theta_{i-1}} \frac{\partial}{\partial \theta_i}. \end{aligned}$$

We only need the radial part of the Laplace operator for the direct calculation of the zero energy Green's function  $G_d(\mathbf{x}, E=0) \equiv G_d(r)$ . The condition

$$\Delta G_d(r) = \frac{1}{r^{d-1}} \frac{d}{dr} r^{d-1} \frac{d}{dr} G_d(r) = -\delta(\mathbf{x})$$

implies after integration over a spherical volume with radius  $r$ ,

$$S_{d-1}r^{d-1} \frac{d}{dr}G_d(r) = \frac{2\sqrt{\pi}^d}{\Gamma(d/2)}r^{d-1} \frac{d}{dr}G_d(r) = -1.$$

This yields

$$G_d(r) = \begin{cases} (a-r)/2, & d = 1, \\ -(2\pi)^{-1} \ln(r/a), & d = 2, \\ \Gamma\left(\frac{d-2}{2}\right) \left(4\sqrt{\pi}^d r^{d-2}\right)^{-1}, & d \geq 3. \end{cases} \tag{J.24}$$

The integration constant determines for  $d = 1$  and  $d = 2$  at which distance  $a$  the Green's function vanishes. For  $d \geq 3$  the vanishing integration constant  $\propto a^{2-d}$  is imposed by the usual boundary condition  $\lim_{r \rightarrow \infty} G_{d \geq 3}(r) = 0$ .

The free Green's function in the  $\mathbf{x}$ -representation with full energy dependence is still translation invariant and isotropic,  $\langle \mathbf{x} | G_d(E) | \mathbf{x}' \rangle \equiv G_d(\mathbf{x} - \mathbf{x}', E) = G_d(|\mathbf{x} - \mathbf{x}'|, E)$ , and can be gotten from integration of the condition

$$\Delta G_d(\mathbf{x}, E) + \frac{2m}{\hbar^2} E G_d(\mathbf{x}, E) = -\delta(\mathbf{x}). \tag{J.25}$$

The result (J.24) motivates an *ansatz*

$$G_d(\mathbf{x}, E) = f_d(r, E)G_d(r). \tag{J.26}$$

This will solve (J.25) if the factor  $f_d(r, E)$  satisfies

$$\frac{d^2}{dr^2}f_d(r, E) + \frac{3-d}{r} \frac{d}{dr}f_d(r, E) + \frac{2m}{\hbar^2} E f_d(r, E) = 0, \quad f_d(0, E) = 1.$$

This yields together with the requirement  $G_d(\mathbf{x}, E)|_{E < 0} \in \mathbb{R}$  and analyticity in  $E$  (and the convention  $\sqrt{-E}|_{E > 0} = -i\sqrt{E}$ ),

$$G_d(\mathbf{x}, E) = \frac{\Theta(-E)}{\sqrt{2\pi}^d} \left( \frac{\sqrt{-2mE}}{\hbar r} \right)^{\frac{d-2}{2}} K_{\frac{d-2}{2}} \left( \sqrt{-2mE} \frac{r}{\hbar} \right) + i \frac{\pi}{2} \frac{\Theta(E)}{\sqrt{2\pi}^d} \left( \frac{\sqrt{2mE}}{\hbar r} \right)^{\frac{d-2}{2}} H_{\frac{d-2}{2}}^{(1)} \left( \sqrt{2mE} \frac{r}{\hbar} \right), \tag{J.27}$$

where the conventions and definitions from [1] were used for the modified Bessel and Hankel functions.

The result (J.27) tells us that outgoing spherical waves of energy  $E > 0$  in  $d$  dimensions are given by Hankel functions,

$$G_d(\mathbf{x}, E > 0) = \frac{i\pi}{2\sqrt{2\pi}^d} \left( \frac{\sqrt{2mE}}{\hbar r} \right)^{\frac{d-2}{2}} H_{\frac{d-2}{2}}^{(1)} \left( \sqrt{2mE} \frac{r}{\hbar} \right),$$

with asymptotic form

$$G_d(\mathbf{x}, E > 0) \Big|_{kr \gg 1} \simeq \frac{1}{2k} \left( \frac{k}{2\pi r} \right)^{\frac{d-1}{2}} \exp\left( ikr - i\frac{d-3}{4}\pi \right),$$

while  $d$ -dimensional Yukawa potentials of range  $a$  are described by modified Bessel functions,

$$V_d(r) = \frac{1}{\sqrt{2\pi}^d r^{d-2}} \left( \frac{r}{a} \right)^{\frac{d-2}{2}} K_{\frac{d-2}{2}} \left( \frac{r}{a} \right),$$

with asymptotic form

$$V_d(r \gg a) \simeq \frac{\exp(-r/a)}{2\sqrt{a}^{d-3} \sqrt{2\pi} r^{d-1}}.$$

The result (J.27) can also be derived through Fourier transformation (J.21) from the energy-dependent retarded Green's function in  $\mathbf{k}$  space,

$$G_d(\mathbf{x}, E) = \frac{1}{(2\pi)^d} \int d^d \mathbf{k} G_d(\mathbf{k}, E) \exp(i\mathbf{k} \cdot \mathbf{x}),$$

$$G_d(\mathbf{k}, E) = \frac{1}{\mathbf{k}^2 - (2mE/\hbar^2) - i\epsilon},$$

or in terms of poles in the complex  $k$  plane (where  $k \equiv |\mathbf{k}|$  for  $d > 1$ ),

$$G_d(\mathbf{k}, E) = \frac{\Theta(E)}{(k - \sqrt{2mE/\hbar^2} - i\epsilon)(k + \sqrt{2mE/\hbar^2} + i\epsilon)} + \frac{\Theta(-E)}{(k - i\sqrt{-2mE/\hbar^2})(k + i\sqrt{-2mE/\hbar^2})}. \quad (\text{J.28})$$

This yields for  $d > 1$  (for the  $\vartheta$  integral see [32], p. 457, no. 6)

$$\begin{aligned}
 G_d(\mathbf{x}, E) &= \frac{S_{d-2}}{(2\pi)^d} \int_0^\infty dk \int_0^\pi d\vartheta \frac{k^{d-1} \exp(ikr \cos \vartheta)}{k^2 - (2mE/\hbar^2) - i\epsilon} \sin^{d-2} \vartheta \\
 &= \frac{1}{2^{d-1} \sqrt{\pi}^{d+1} \Gamma(\frac{d-1}{2})} \int_0^\infty dk \int_0^\pi d\vartheta \frac{k^{d-1} \exp(ikr \cos \vartheta)}{k^2 - (2mE/\hbar^2) - i\epsilon} \sin^{d-2} \vartheta \\
 &= \frac{1}{\sqrt{2\pi}^d \sqrt{r}^{d-2}} \int_0^\infty dk \frac{\sqrt{k}^d}{k^2 - (2mE/\hbar^2) - i\epsilon} J_{\frac{d-2}{2}}(kr) \\
 &= \frac{\Theta(-E)}{\sqrt{2\pi}^d} \left( \frac{\sqrt{-2mE}}{\hbar r} \right)^{\frac{d-2}{2}} K_{\frac{d-2}{2}} \left( \sqrt{-2mE} \frac{r}{\hbar} \right) \\
 &\quad + i \frac{\pi}{2} \frac{\Theta(E)}{\sqrt{2\pi}^d} \left( \frac{\sqrt{2mE}}{\hbar r} \right)^{\frac{d-2}{2}} H_{\frac{d-2}{2}}^{(1)} \left( \sqrt{2mE} \frac{r}{\hbar} \right). \tag{J.29}
 \end{aligned}$$

For the  $k$  integral for  $E > 0$  see [33], p. 179, no. 28. The real part of the integral for  $E < 0$  is given on p. 179, no. 35. The integrals can also be performed with symbolic computation programs, of course. The  $k$  integral actually diverges for  $d \geq 5$ , but recall that we have found the same solution for arbitrary  $d$  from the *ansatz* (J.26). Fourier transformation of (J.28) for  $d = 1$  directly yields the result (20.6), which also coincides with (J.29) for  $d = 1$ .

### The time evolution operator in various representations

We have seen that the Green's function  $\mathcal{G}_{d,v}(t)$  in the time domain is intimately connected to the time evolution operator

$$U(t) = \exp(-iHt/\hbar)$$

through equations (J.12, J.13). We can also define an energy representation for the time evolution operator in analogy to equations (J.9, J.10),

$$U(E) = \int_{-\infty}^\infty dt U(t) \exp(iEt/\hbar) = 2\pi\hbar\delta(E - H). \tag{J.30}$$

Indeed, we have encountered this representation of the time evolution operator already in the frequency decomposition (5.14) of states,

$$|\psi(\omega)\rangle = \sqrt{2\pi} U(\hbar\omega) |\psi(t = 0)\rangle.$$

The free  $d$ -dimensional evolution operator in the time domain is simply the product of  $d$  one-dimensional evolution operators,

$$U_0(t) = \exp\left(-\frac{it}{2m\hbar}\mathbf{p}^2\right),$$

$$\langle \mathbf{k} | U_0(t) | \mathbf{k}' \rangle = U_0(\mathbf{k}, t) \delta(\mathbf{k} - \mathbf{k}'), \quad U_0(\mathbf{k}, t) = \exp\left(-i\frac{\hbar t}{2m}\mathbf{k}^2\right),$$

$$\langle \mathbf{x} | U_0(t) | \mathbf{k} \rangle = \frac{1}{\sqrt{2\pi}^d} \exp\left(i\mathbf{k} \cdot \mathbf{x} - i\frac{\hbar t}{2m}\mathbf{k}^2\right),$$

and

$$\langle \mathbf{x} | U_0(t) | \mathbf{x}' \rangle = \frac{1}{(2\pi)^d} \int d^3\mathbf{k} \exp[i\mathbf{k} \cdot (\mathbf{x} - \mathbf{x}')] U_0(\mathbf{k}, t) = U_0(\mathbf{x} - \mathbf{x}', t),$$

$$U_0(\mathbf{x}, t) = \sqrt{\frac{m^{-d}}{2\pi i\hbar t}} \exp\left(i\frac{m\mathbf{x}^2}{2\hbar t}\right).$$

Just like for the free Green's functions, the dependence on  $d$  becomes more interesting in the energy domain. The equation

$$U_0(\mathbf{k}, E) = 2\pi\hbar\delta\left(E - \frac{\hbar^2\mathbf{k}^2}{2m}\right) = \pi\sqrt{\frac{2m}{E}}\delta\left(|\mathbf{k}| - \frac{\sqrt{2mE}}{\hbar}\right)$$

yields

$$\begin{aligned} U_0(\mathbf{x}, E) &= \frac{1}{(2\pi)^d} \int d^d\mathbf{k} \exp(i\mathbf{k} \cdot \mathbf{x}) U_0(\mathbf{k}, E) \\ &= \frac{\Theta(E) S_{d-2}}{2^d (\pi\hbar)^{d-1}} \sqrt{2m^d} \sqrt{E}^{d-2} \int_0^\pi d\vartheta \exp\left(i\sqrt{2mE} \frac{r}{\hbar} \cos\vartheta\right) \sin^{d-2}\vartheta \\ &= \Theta(E) \frac{m}{\hbar} \left(\frac{1}{\pi\hbar r} \sqrt{\frac{mE}{2}}\right)^{\frac{d-2}{2}} J_{\frac{d-2}{2}}\left(\sqrt{2mE} \frac{r}{\hbar}\right). \end{aligned} \quad (\text{J.31})$$

We have encountered several incarnations of the time evolution equation

$$|\psi(t)\rangle = U_0(t - t') |\psi(t')\rangle,$$

e.g. with  $\langle \mathbf{k} | \psi \rangle \equiv \langle \mathbf{k} | \psi(0) \rangle$ ,

$$\begin{aligned} \langle \mathbf{x} | \psi(t) \rangle &= \int d^d\mathbf{k} \langle \mathbf{x} | U_0(t) | \mathbf{k} \rangle \langle \mathbf{k} | \psi \rangle \\ &= \frac{1}{\sqrt{2\pi}^d} \int d^d\mathbf{k} \exp\left[i\left(\mathbf{k} \cdot \mathbf{x} - \frac{\hbar t}{2m}\mathbf{k}^2\right)\right] \psi(\mathbf{k}) \\ &= \int d^d\mathbf{x}' U_0(\mathbf{x} - \mathbf{x}', t - t') \langle \mathbf{x}' | \psi(t') \rangle. \end{aligned}$$

Equation (J.31) implies with  $|\psi\rangle \equiv |\psi(t = 0)\rangle$  the  $(\mathbf{x}, \omega)$  representation for free states in terms of their  $(\mathbf{x}, t = 0)$  representations,

$$\begin{aligned}
 \langle \mathbf{x} | \psi(\omega) \rangle &= \frac{1}{\sqrt{2\pi}} \int dt \exp(i\omega t) \langle \mathbf{x} | \psi(t) \rangle \\
 &= \frac{1}{\sqrt{2\pi}} \int d^d \mathbf{x}' \int dt \exp(i\omega t) \langle \mathbf{x} | U_0(t) | \mathbf{x}' \rangle \langle \mathbf{x}' | \psi \rangle \\
 &= \frac{1}{\sqrt{2\pi}} \int d^d \mathbf{x}' \langle \mathbf{x} | U_0(\hbar\omega) | \mathbf{x}' \rangle \langle \mathbf{x}' | \psi \rangle \\
 &= \Theta(\omega) \frac{m}{\sqrt{2\pi\hbar}} \left( \frac{1}{\pi} \sqrt{\frac{m\omega}{2\hbar}} \right)^{\frac{d-2}{2}} \\
 &\quad \times \int d^d \mathbf{x}' J_{\frac{d-2}{2}} \left( \sqrt{\frac{2m\omega}{\hbar}} |\mathbf{x} - \mathbf{x}'| \right) \frac{\langle \mathbf{x}' | \psi \rangle}{\sqrt{|\mathbf{x} - \mathbf{x}'|^{d-2}}}. \tag{J.32}
 \end{aligned}$$

In turn, equation (5.12) implies for the initial state

$$|\psi\rangle = \frac{1}{\sqrt{2\pi}} \int d\omega |\psi(\omega)\rangle,$$

and therefore the kernel in (J.32) must yield a  $d$ -dimensional  $\delta$  function,

$$\frac{m}{\sqrt{2\pi}^d \hbar} \int_0^\infty d\omega \left( \sqrt{\frac{2m\omega}{\hbar}} \frac{1}{|\mathbf{x}|} \right)^{\frac{d-2}{2}} J_{\frac{d-2}{2}} \left( \sqrt{\frac{2m\omega}{\hbar}} |\mathbf{x}| \right) = \delta(\mathbf{x}),$$

or in terms of magnitude of wave number,

$$\frac{1}{\sqrt{2\pi}^d} \int_0^\infty dk k \left( \frac{k}{r} \right)^{\frac{d-2}{2}} J_{\frac{d-2}{2}}(kr) = \delta(\mathbf{x}). \tag{J.33}$$

However, this is just the familiar relation

$$\frac{1}{(2\pi)^d} \int d^d \mathbf{k} \exp(i\mathbf{k} \cdot \mathbf{x}) = \delta(\mathbf{x})$$

after evaluation of the angular integrals in polar coordinates in  $\mathbf{k}$  space.

In particular, for  $d = 1$  we find

$$\langle x | \psi(\omega) \rangle = \Theta(\omega) \sqrt{\frac{m}{\pi\hbar\omega}} \int dx' \cos\left( \sqrt{\frac{2m\omega}{\hbar}} (x - x') \right) \langle x' | \psi \rangle. \tag{J.34}$$

In two dimensions we find

$$\langle \mathbf{x} | \psi(\omega) \rangle = \Theta(\omega) \frac{m}{\sqrt{2\pi\hbar}} \int d^2 \mathbf{x}' J_0 \left( \sqrt{\frac{2m\omega}{\hbar}} |\mathbf{x} - \mathbf{x}'| \right) \langle \mathbf{x}' | \psi \rangle, \quad (\text{J.35})$$

and in three dimensions we find

$$\langle \mathbf{x} | \psi(\omega) \rangle = \Theta(\omega) \frac{m}{\sqrt{2\pi^3\hbar}} \int d^3 \mathbf{x}' \sin \left( \sqrt{\frac{2m\omega}{\hbar}} |\mathbf{x} - \mathbf{x}'| \right) \frac{\langle \mathbf{x}' | \psi \rangle}{|\mathbf{x} - \mathbf{x}'|}. \quad (\text{J.36})$$

The free states in the  $(\mathbf{x}, \omega)$  representation are a superposition of stationary radial waves, where each point contributes with weight  $\langle \mathbf{x}' | \psi \rangle$ .

## Relativistic Green's functions in $d$ spatial dimensions

Although the theory in this subsection is relativistic, we will not use manifestly Lorentz covariant 4-vector notation like  $x = (ct, \mathbf{x})$ ,  $k = (\omega/c, \mathbf{k})$  for the space-time and momentum variables because we are also interested in mixed representations of the Green's functions like  $G(\mathbf{x}, \omega)$ . For the manifestly covariant notation see the note at the end of this Appendix.

The relativistic free scalar Green's function in the time domain must satisfy

$$\left( \Delta - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{m^2 c^2}{\hbar^2} \right) G_d(\mathbf{x}, t; \mathbf{x}', t') = -\delta(\mathbf{x} - \mathbf{x}') \delta(t - t'). \quad (\text{J.37})$$

This yields after transformation into  $(\mathbf{k}, \omega)$  space

$$G_d(\mathbf{k}, \omega; \mathbf{k}', \omega') = G_d(\mathbf{k}, \omega) \delta(\mathbf{k} - \mathbf{k}') \delta(\omega - \omega'), \quad (\text{J.38})$$

where the factor  $G_d(\mathbf{k}, \omega)$  is

$$G_d(\mathbf{k}, \omega) = \frac{1}{\mathbf{k}^2 - \frac{\omega^2}{c^2} + \frac{m^2 c^2}{\hbar^2} - i\epsilon}. \quad (\text{J.39})$$

The shift  $-i\epsilon$ ,  $\epsilon > 0$ , into the complex plane is such that this reproduces the retarded non-relativistic Green's function (J.19) in the non-relativistic limit

$$\omega \Rightarrow \frac{mc^2 + E}{\hbar},$$

when terms of order  $\mathcal{O}(E^2)$  are neglected. However, in the relativistic case this yields both retarded and advanced contributions in the time domain. This convention for

the poles in the relativistic theory was introduced by Richard Feynman<sup>2</sup> and yields the Green's functions of Stückelberg and Feynman.

The solution in  $x = (ct, \mathbf{x})$  space is then

$$G_d(\mathbf{x}, t; \mathbf{x}', t') = G_d(\mathbf{x} - \mathbf{x}', t - t'),$$

$$G_d(\mathbf{x}, t) = \frac{1}{2\pi} \int d\omega G_d(\mathbf{x}, \omega) \exp(-i\omega t), \tag{J.40}$$

$$G_d(\mathbf{x}, \omega) = \frac{1}{(2\pi)^d} \int d^d\mathbf{k} G_d(\mathbf{k}, \omega) \exp(i\mathbf{k} \cdot \mathbf{x}). \tag{J.41}$$

The integral is the same as in (J.29) with the substitution

$$\frac{2m}{\hbar^2} E \rightarrow \frac{\omega^2}{c^2} - \frac{m^2 c^2}{\hbar^2},$$

i.e.

$$G_d(\mathbf{x}, \omega) = \frac{\Theta(mc^2 - \hbar|\omega|)}{\sqrt{2\pi}^d} \left( \frac{\sqrt{m^2 c^4 - \hbar^2 \omega^2}}{\hbar c r} \right)^{\frac{d-2}{2}}$$

$$\times K_{\frac{d-2}{2}} \left( \sqrt{m^2 c^4 - \hbar^2 \omega^2} \frac{r}{\hbar c} \right)$$

$$+ i \frac{\pi}{2} \frac{\Theta(\hbar|\omega| - mc^2)}{\sqrt{2\pi}^d} \left( \frac{\sqrt{\hbar^2 \omega^2 - m^2 c^4}}{\hbar c r} \right)^{\frac{d-2}{2}}$$

$$\times H_{\frac{d-2}{2}}^{(1)} \left( \sqrt{\hbar^2 \omega^2 - m^2 c^4} \frac{r}{\hbar c} \right). \tag{J.42}$$

The  $\omega = 0$  Green's functions

$$\left( \Delta - \frac{m^2 c^2}{\hbar^2} \right) G_d(\mathbf{x}) = -\delta(\mathbf{x}), \quad G_d(\mathbf{x}) = \frac{1}{\sqrt{2\pi}^d} \left( \frac{mc}{\hbar r} \right)^{\frac{d-2}{2}} K_{\frac{d-2}{2}} \left( \frac{mc}{\hbar} r \right),$$

yield again the results (J.24) in the limit  $m \rightarrow 0$ , albeit with diverging integration constants in low dimensions,

$$a_{d=1} = \frac{\hbar}{mc}, \quad a_{d=2} = \frac{2\hbar}{mc} \exp(-\gamma).$$

In terms of poles in the complex  $k$  plane, the complex shift in (J.39) implies

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<sup>2</sup>R.P. Feynman, Phys. Rev. 76, 749 (1949).

$$G_d(\mathbf{k}, \omega) = \frac{c^2 \Theta(\hbar\omega - mc^2)}{\left(ck - \sqrt{\omega^2 - (mc^2/\hbar)^2} - i\epsilon\right) \left(ck + \sqrt{\omega^2 - (mc^2/\hbar)^2} + i\epsilon\right)} + \frac{c^2 \Theta(mc^2 - \hbar\omega)}{\left(ck - i\sqrt{(mc^2/\hbar)^2 - \omega^2}\right) \left(ck - i\sqrt{(mc^2/\hbar)^2 - \omega^2}\right)}. \quad (\text{J.43})$$

However, in terms of poles in the complex  $\omega$  plane, equation (J.39) implies

$$G_d(\mathbf{k}, \omega) = -\frac{c^2}{\left(\omega - c\sqrt{k^2 + (mc/\hbar)^2} + i\epsilon\right) \left(\omega + c\sqrt{k^2 + (mc/\hbar)^2} - i\epsilon\right)}.$$

Fourier transformation to the time domain therefore yields a representation of the relativistic free Green's function which explicitly shows the combination of retarded positive frequency and advanced negative frequency components,

$$G_d(\mathbf{k}, t) = \frac{1}{2\pi} \int d\omega G_d(\mathbf{k}, \omega) \exp(-i\omega t) = ic\Theta(t) \frac{\exp\left(-i\sqrt{k^2 + (mc/\hbar)^2} ct\right)}{2\sqrt{k^2 + (mc/\hbar)^2}} + ic\Theta(-t) \frac{\exp\left(i\sqrt{k^2 + (mc/\hbar)^2} ct\right)}{2\sqrt{k^2 + (mc/\hbar)^2}}. \quad (\text{J.44})$$

On the other hand, shifting both poles into the lower complex  $\omega$  plane,

$$G_d^{(r)}(\mathbf{k}, \omega) = -\frac{c^2}{\left(\omega - c\sqrt{k^2 + (mc/\hbar)^2} + i\epsilon\right) \left(\omega + c\sqrt{k^2 + (mc/\hbar)^2} + i\epsilon\right)},$$

yields the retarded relativistic Green's function

$$G_d^{(r)}(\mathbf{k}, t) = \frac{1}{2\pi} \int d\omega G_d^{(r)}(\mathbf{k}, \omega) \exp(-i\omega t) = c\Theta(t) \frac{\sin\left(\sqrt{k^2 + (mc/\hbar)^2} ct\right)}{\sqrt{k^2 + (mc/\hbar)^2}} = c^2 \Theta(t) \mathcal{K}_d(\mathbf{k}, t), \quad (\text{J.45})$$

cf. equation (21.9). If  $\mathcal{K}_d(\mathbf{x}, t)$  exists, then one can easily verify that the properties

$$\left( \Delta - \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{m^2 c^2}{\hbar^2} \right) \mathcal{K}_d(\mathbf{x}, t) = 0,$$

$$\mathcal{K}_d(\mathbf{x}, 0) = 0, \quad \left. \frac{\partial}{\partial t} \mathcal{K}_d(\mathbf{x}, t) \right|_{t=0} = \delta(\mathbf{x})$$

imply that  $G_d^{(r)}(\mathbf{x}, t) = c^2 \Theta(t) \mathcal{K}_d(\mathbf{x}, t)$  is a retarded Green's function.

On the other hand, shifting both poles into the upper complex  $\omega$  plane,

$$G_d^{(a)}(\mathbf{k}, \omega) = - \frac{c^2}{\left( \omega - c \sqrt{k^2 + (mc/\hbar)^2} - i\epsilon \right) \left( \omega + c \sqrt{k^2 + (mc/\hbar)^2} - i\epsilon \right)},$$

yields the advanced relativistic free Green's function

$$\begin{aligned} G_d^{(a)}(\mathbf{k}, t) &= \frac{1}{2\pi} \int d\omega G_d^{(a)}(\mathbf{k}, \omega) \exp(-i\omega t) \\ &= -c \Theta(-t) \frac{\sin\left(\sqrt{k^2 + (mc/\hbar)^2} ct\right)}{\sqrt{k^2 + (mc/\hbar)^2}} \\ &= -c^2 \Theta(-t) \mathcal{K}_d(\mathbf{k}, t) = G_d^{(r)}(\mathbf{k}, -t). \end{aligned} \tag{J.46}$$

### Retarded relativistic Green's functions in $(\mathbf{x}, t)$ representation

Evaluation of the Green's functions  $G_d^{(r)}(\mathbf{x}, t)$  and  $G_d(\mathbf{x}, t)$  for the massive Klein-Gordon equation is very cumbersome if one uses standard Fourier transformation between time and frequency. It is much more convenient to use Fourier transformation with imaginary frequency, which is known as Laplace transformation. We will demonstrate this for the retarded Green's function. We try a Laplace transform of  $G_d^{(r)}(\mathbf{x}, t)$  in the form<sup>3</sup>

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<sup>3</sup>Assuming only  $\Re w \geq 0$  assumes that the retarded Green's functions are integrable along the time axis. This makes physical sense since the impact of a perturbation which occurred at time  $t' = 0$  at the point  $\mathbf{x}' = 0$  that is felt at the point  $\mathbf{x}$  should decrease with time. The assumption can also be justified *a posteriori* from the explicit results (J.58–J.60), which show that the Green's functions for  $d \leq 3$  oscillate and decay for  $t \rightarrow \infty$ . For Laplace transforms of less well behaved functions  $G(\mathbf{x}, t)$  one can require  $\Re w > \nu$  if  $\exp(-\nu t)G(\mathbf{x}, t)$  is bounded for  $t \rightarrow \infty$ . The vertical integration contour for the inverse transformation (J.48) must then be to the right of  $\nu - i\infty \rightarrow \nu + i\infty$ .

$$g_d(\mathbf{x}, w) = \int_0^\infty dt \exp(-wt) G_d^{(r)}(\mathbf{x}, t), \quad \Re w \geq 0. \quad (\text{J.47})$$

The completeness relation for Fourier monomials,

$$\delta(t) = \frac{1}{2\pi} \int_{-\infty}^\infty d\omega \exp(-i\omega t) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d\omega \exp(\omega t)$$

then yields the inversion of (J.47),

$$G_d^{(r)}(\mathbf{x}, t) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} d\omega \exp(\omega t) g_d(\mathbf{x}, \omega). \quad (\text{J.48})$$

The condition (J.37) on the  $d$ -dimensional scalar Green's functions then implies

$$\left( \Delta - \frac{w^2}{c^2} - \frac{m^2 c^2}{\hbar^2} \right) g_d(\mathbf{x}, w) = -\delta(\mathbf{x}) \quad (\text{J.49})$$

with solution

$$g_d(\mathbf{x}, w) = \frac{1}{(2\pi)^d} \int d^d \mathbf{k} \frac{\exp(i\mathbf{k} \cdot \mathbf{x})}{k^2 + (w/c)^2 + (mc/\hbar)^2}.$$

In one dimension this yields

$$g_1(x, w) = \frac{c \exp\left(-\sqrt{w^2 + (mc^2/\hbar)^2} |x|/c\right)}{2\sqrt{w^2 + (mc^2/\hbar)^2}}. \quad (\text{J.50})$$

In higher dimensions, we need to calculate

$$\begin{aligned} g_d(\mathbf{x}, w) &= \frac{S_{d-2}}{(2\pi)^d} \int_0^\infty dk \int_0^\pi d\vartheta k^{d-1} \sin^{d-2} \vartheta \frac{\exp(ikr \cos \vartheta)}{k^2 + (w/c)^2 + (mc/\hbar)^2} \\ &= \frac{1}{\sqrt{2\pi}^d} \int_0^\infty dk \frac{k^{d-1}}{k^2 + (w/c)^2 + (mc/\hbar)^2} \frac{1}{\sqrt{kr}} J_{\frac{d-2}{2}}(kr). \end{aligned} \quad (\text{J.51})$$

We can formally reduce (J.51) for  $d \geq 3$  to the corresponding integrals in lower dimensions by using the relation

$$\left( -\frac{1}{x} \frac{d}{dx} \right)^n \frac{J_\nu(x)}{x^\nu} = \frac{J_{\nu+n}(x)}{x^{\nu+n}},$$

---

However, this would not save the day for the non-existent functions  $G_{d \geq 4}^{(r)}(\mathbf{x}, t)$ , although we can find functions  $g_d(\mathbf{x}, w)$  (J.54, J.55) for every number  $d$  of dimensions.

see number 9.1.30, p. 361 in [1]. This yields for  $d = 2n + 1$

$$\begin{aligned} \frac{1}{\sqrt{kr}^{d-2}} J_{\frac{d-2}{2}}(kr) &= k^{-2n} \left( -\frac{1}{r} \frac{\partial}{\partial r} \right)^n \sqrt{kr} J_{-\frac{1}{2}}(kr) \\ &= \sqrt{\frac{2}{\pi}} k^{-2n} \left( -\frac{1}{r} \frac{\partial}{\partial r} \right)^n \cos(kr), \end{aligned} \tag{J.52}$$

and for  $d = 2n + 2$ ,

$$\frac{1}{\sqrt{kr}^{d-2}} J_{\frac{d-2}{2}}(kr) = k^{-2n} \left( -\frac{1}{r} \frac{\partial}{\partial r} \right)^n J_0(kr). \tag{J.53}$$

The resulting relations for the Green's functions in the  $(\mathbf{x}, w)$  representations are then

$$\begin{aligned} g_{2n+1}(\mathbf{x}, w) &= \left( -\frac{1}{2\pi r} \frac{\partial}{\partial r} \right)^n \frac{1}{\pi} \int_0^\infty dk \frac{\cos(kr)}{k^2 + (w/c)^2 + (mc/\hbar)^2} \\ &= \left( -\frac{1}{2\pi r} \frac{\partial}{\partial r} \right)^n \frac{c \exp\left(-\sqrt{w^2 + (mc^2/\hbar)^2} r/c\right)}{2\sqrt{w^2 + (mc^2/\hbar)^2}}, \end{aligned} \tag{J.54}$$

and

$$\begin{aligned} g_{2n+2}(\mathbf{x}, w) &= \left( -\frac{1}{2\pi r} \frac{\partial}{\partial r} \right)^n \frac{1}{\pi} \int_0^\infty dk \frac{k J_0(kr)}{k^2 + (w/c)^2 + (mc/\hbar)^2} \\ &= \left( -\frac{1}{2\pi r} \frac{\partial}{\partial r} \right)^n \frac{1}{2\pi} K_0\left(\sqrt{w^2 + (mc^2/\hbar)^2} \frac{r}{c}\right). \end{aligned} \tag{J.55}$$

Inverse Laplace transformation yields the retarded Green's functions  $G_d^{(r)}(\mathbf{x}, t)$ ,

$$G_{2n+1}^{(r)}(\mathbf{x}, t) = \left( -\frac{1}{2\pi r} \frac{\partial}{\partial r} \right)^n \frac{c}{2} \Theta(ct - r) J_0\left(mc\sqrt{c^2 t^2 - r^2}/\hbar\right), \tag{J.56}$$

$$G_{2n+2}^{(r)}(\mathbf{x}, t) = \left( -\frac{1}{2\pi r} \frac{\partial}{\partial r} \right)^n \frac{c}{2\pi} \frac{\Theta(ct - r)}{\sqrt{c^2 t^2 - r^2}} \cos\left(mc\sqrt{c^2 t^2 - r^2}/\hbar\right). \tag{J.57}$$

We note that the retarded Green's functions for fixed  $r$  decrease like  $t^{-(n+1)} = t^{-\lfloor(d+1)/2\rfloor}$  for  $t \rightarrow \infty$ , except the  $\delta$  function singularities become unacceptable for  $d \geq 4$ .

The retarded relativistic Green's functions in one, two and three dimensions are therefore

$$G_1^{(r)}(x, t) = \frac{c}{2} \Theta(ct - |x|) J_0\left(mc\sqrt{c^2 t^2 - x^2}/\hbar\right), \tag{J.58}$$

$$G_2^{(r)}(\mathbf{x}, t) = \frac{c}{2\pi} \frac{\Theta(ct - r)}{\sqrt{c^2 t^2 - r^2}} \cos\left(mc\sqrt{c^2 t^2 - r^2}/\hbar\right), \quad (\text{J.59})$$

and

$$G_3^{(r)}(\mathbf{x}, t) = \frac{c}{4\pi r} \delta(r - ct) - \frac{mc^2}{4\pi\hbar} \frac{\Theta(ct - r)}{\sqrt{c^2 t^2 - r^2}} J_1\left(mc\sqrt{c^2 t^2 - r^2}/\hbar\right). \quad (\text{J.60})$$

The  $(\mathbf{x}, t)$  representations of the corresponding advanced Green's functions then follow from (J.46) as

$$G_d^{(a)}(\mathbf{x}, t) = G_d^{(r)}(\mathbf{x}, -t).$$

The propagator function  $\mathcal{K}_d(\mathbf{x}, t)$  for the free Klein-Gordon fields follows from (J.45, J.46) as

$$c^2 \mathcal{K}_d(\mathbf{x}, t) = G_d^{(r)}(\mathbf{x}, t) - G_d^{(a)}(\mathbf{x}, t). \quad (\text{J.61})$$

The functions  $G_{d \geq 4}^{(r)}(\mathbf{x}, t)$  and  $\mathcal{K}_{d \geq 4}(\mathbf{x}, t)$  do not exist, but the corresponding functions  $G_d^{(r)}(\mathbf{k}, t) = c^2 \Theta(t) \mathcal{K}_d(\mathbf{k}, t)$  (J.45) and  $G_d^{(r)}(\mathbf{k}, \omega)$  exist in any number of dimensions.

## Green's functions for Dirac operators in $d$ dimensions

We now restore summation convention. The Green's functions for the free Dirac operator must satisfy

$$\left(i\gamma^\mu \partial_\mu - \frac{mc}{\hbar}\right) S_d(\mathbf{x}, t) = -\delta(\mathbf{x})\delta(t). \quad (\text{J.62})$$

Since the Dirac operator is a factor of the Klein-Gordon operator, the solutions of the equations (J.62) and (J.37) are related by

$$S_d(\mathbf{x}, t) = \left(i\gamma^\mu \partial_\mu + \frac{mc}{\hbar}\right) G_d(\mathbf{x}, t) \quad (\text{J.63})$$

and

$$\begin{aligned} G_d(\mathbf{x}, t) &= \int d^d \mathbf{x}' \int dt' S_d(\mathbf{x}' - \mathbf{x}, t' - t) \cdot S_d(\mathbf{x}', t') \\ &= \int d^d \mathbf{x}' \int dt' S_d(\mathbf{x}', t') \cdot S_d(\mathbf{x}' + \mathbf{x}, t' + t). \end{aligned} \quad (\text{J.64})$$

The free Dirac Green's function in wave number representation is (here  $k^2 \equiv k^\mu k_\mu$ )

$$S_d(k) = \hbar \frac{mc - \hbar \gamma^\mu k_\mu}{\hbar^2 k^2 + m^2 c^2 - i\epsilon}, \quad (\text{J.65})$$

where the pole shifts again correspond to the Feynman propagator with retarded and advanced components.

## Green's functions in covariant notation

The relativistic free scalar Green's function satisfies

$$\frac{p^2 + m^2 c^2}{\hbar^2} G_d = 1, \quad (\text{J.66})$$

i.e. in the  $k = (\omega/c, \mathbf{k})$  domain

$$\langle k | G_d | k' \rangle = G_d(k) \delta(k - k'), \quad (\text{J.67})$$

where the factor  $G_d(k)$  is

$$G_d(k) = \frac{1}{k^2 + (m^2 c^2 / \hbar^2) - i\epsilon}. \quad (\text{J.68})$$

This yields after transformation into  $x = (ct, \mathbf{x})$  space ( $D = d + 1$ ),

$$\begin{aligned} \langle x | G_d | x' \rangle &= \frac{1}{(2\pi)^D} \int d^D k \int d^D k' \langle k | G_d | k' \rangle \exp[i(k \cdot x - k' \cdot x')], \\ &= \frac{1}{(2\pi)^D} \int d^D k G_d(k) \exp[ik \cdot (x - x')] = G_d(x - x'), \end{aligned} \quad (\text{J.69})$$

which satisfies

$$\left( \partial^2 - \frac{m^2 c^2}{\hbar^2} \right) \langle x | G_d | x' \rangle = \left( \partial'^2 - \frac{m^2 c^2}{\hbar^2} \right) \langle x | G_d | x' \rangle = -\delta(x - x'). \quad (\text{J.70})$$

The relation to (J.37–J.60) is

$$\begin{aligned} \langle x | G_d | x' \rangle &= \frac{1}{c} G_d(\mathbf{x}, t; \mathbf{x}', t'), \quad \langle k | G_d | k' \rangle = c G_d(\mathbf{k}, \omega; \mathbf{k}', \omega'), \\ G_d(k) &= G_d(\mathbf{k}, \omega). \end{aligned}$$

Translation invariance (J.67, J.69) implies that the Green's function in mixed representation is proportional to plane waves,  $\langle x|G_d|k\rangle = G_d(k)\langle x|k\rangle$ .

The fermionic Green's function satisfies

$$\frac{\gamma \cdot p + mc}{\hbar} S_d = 1, \quad S_d = \frac{mc - \gamma \cdot p}{\hbar} G_d, \quad (\text{J.71})$$

or in various representations,

$$\left( i\gamma \cdot \partial - \frac{mc}{\hbar} \right) \langle x|S_d|x'\rangle = -\delta(x - x'), \quad (\text{J.72})$$

$$\langle k|S_d|k'\rangle = S_d(k)\delta(k - k'), \quad \langle x|S_d|k\rangle = S_d(k)\langle x|k\rangle, \quad (\text{J.73})$$

$$S_d(k) = \left( \frac{mc}{\hbar} - \gamma \cdot k \right) G_d(k) = \frac{(mc/\hbar) - \gamma \cdot k}{k^2 + (m^2 c^2/\hbar^2) - i\epsilon}, \quad (\text{J.74})$$

$$\begin{aligned} \langle x|S_d|x'\rangle &= S_d(x - x') = \frac{1}{c} S_d(\mathbf{x} - \mathbf{x}', t - t') \\ &= \frac{1}{(2\pi)^D} \int d^D k S_d(k) \exp[ik \cdot (x - x')] \\ &= \left( i\gamma \cdot \partial + \frac{mc}{\hbar} \right) G_d(x - x'). \end{aligned} \quad (\text{J.75})$$

The pole shifts in (J.68, J.74) correspond to the Feynman conventions. For the retarded Green's functions  $G_d^{(r)}$  and  $S_d^{(r)}$  both poles have to be shifted into the lower  $k^0$  plane. Note that as a consequence of (J.75) the fermionic Green's function also satisfies

$$i\partial'_\mu S_d(x - x')\gamma^\mu + \frac{mc}{\hbar} S_d(x - x') = \delta(x - x'). \quad (\text{J.76})$$

## Green's functions as reproducing kernels

Suppose that  $\mathcal{V}$  is a  $(d + 1)$ -dimensional spacetime volume with boundary  $\partial\mathcal{V}$ . The equation (J.70) and the Klein-Gordon equation imply for a free field  $\phi(x)$  and for  $x$  in  $\mathcal{V}$  the relation

$$\begin{aligned} \phi(x) &= \int_{\mathcal{V}} d^D x' \phi(x') \left( \frac{m^2 c^2}{\hbar^2} - \partial'^2 \right) G_d(x - x') \\ &= \int_{\mathcal{V}} d^D x' \partial'^\mu \left[ G_d(x - x') \overleftrightarrow{\partial}'_\mu \phi(x') \right]. \end{aligned}$$

The Gauss theorem in  $D$  spacetime dimensions then yields a representation for all values of  $\phi(x)$  inside of  $\mathcal{V}$  in terms of the values of the Klein-Gordon field on the boundary  $\partial\mathcal{V}$ ,

$$\phi(x) = \int_{\partial\mathcal{V}} d^d x' n^\mu \left[ G_d(x-x') \overleftrightarrow{\partial}'_\mu \phi(x') \right], \tag{J.77}$$

where  $n^\mu$  is an outward bound normal vector with  $n_0 = 1$  on spacelike boundaries  $t' = \text{constant}$ ,  $t' > t$ , and  $n_0 = -1$  on  $t' = \text{constant}$ ,  $t' < t$ . If  $G_d(x-x')$  is in particular the retarded Green's function,

$$G_d^{(r)}(x-x') = c\Theta(t-t')\mathcal{K}_d(\mathbf{x}-\mathbf{x}', t-t'), \tag{J.78}$$

or the advanced Green's function,

$$G_d^{(a)}(x-x') = c\Theta(t'-t)\mathcal{K}_d(\mathbf{x}-\mathbf{x}', t'-t), \tag{J.79}$$

and  $\partial\mathcal{V}$  contains only the spacelike surface  $t' < t$ , or only the spacelike surface  $t' > t$ , then (J.77) is the solution (21.8) of the initial value problem ( $t' < t$ ) or future value problem<sup>4</sup> ( $t' > t$ ) for the Klein-Gordon field.

For free Dirac fields the Dirac equation and (J.76) implies for  $x \in \mathcal{V}$  the equation

$$\psi(x) = i \int_{\partial\mathcal{V}} d^d x' n_\mu S_d(x-x') \gamma^\mu \psi(x'). \tag{J.80}$$

This yields again the initial/final value solution (21.64) if  $\partial\mathcal{V}$  contains only the spacelike surface  $t' < t$  or only the spacelike surface  $t' > t$ , since the retarded and advanced Green's functions are related to the time evolution kernel (21.65) through

$$\begin{aligned} S_d^{(r)}(x-x') &= i\Theta(t-t')\mathcal{W}_d(\mathbf{x}-\mathbf{x}', t-t')\gamma^0, \\ S_d^{(a)}(x-x') &= -i\Theta(t'-t)\mathcal{W}_d(\mathbf{x}-\mathbf{x}', t-t')\gamma^0, \end{aligned}$$

see also equations (J.75), (J.78), (J.79) and (21.67).

## Liénard-Wiechert potentials in low dimensions

The massless retarded Green's functions solve the basic electromagnetic wave equation for the electromagnetic potentials in Lorentz gauge,

---

<sup>4</sup>The future value problem or backwards evolution problem asks the question: Which field configuration  $\phi(x)$  at time  $t$  yields the prescribed field configuration  $\phi(x')$  at time  $t' > t$  through time evolution with the equations of motion?

$$\left( \partial_\mu \partial^\mu - \frac{m^2 c^2}{\hbar^2} \right) A^\nu(x) = -\mu_0 j^\nu(x), \quad \partial_\mu A^\mu(x) = 0,$$

$$A^\mu(x) = \mu_0 \int d^{d+1}x' G_d^{(r)}(x-x') j^\mu(x').$$

In three dimensions this yields the familiar Liénard-Wiechert potentials from the contributions of the currents on the backward light cone of the spacetime point  $x$ ,

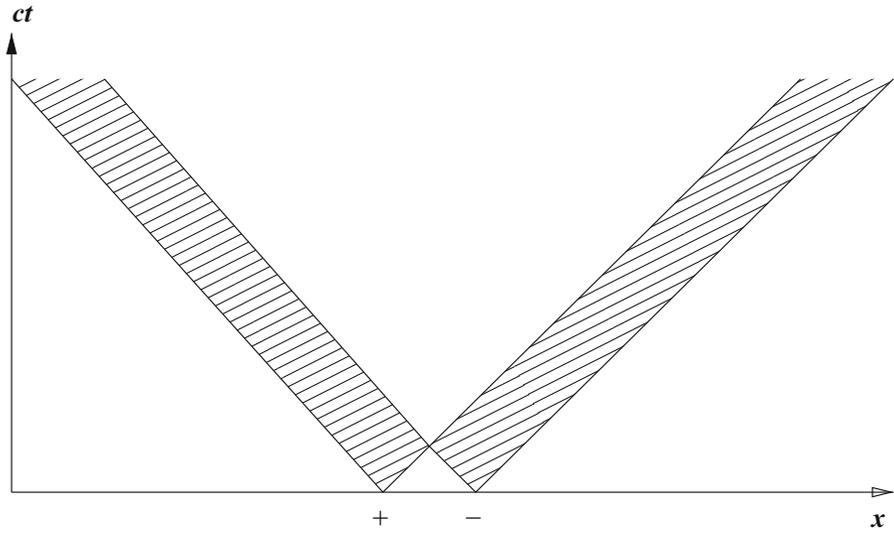
$$A_{d=3}^\mu(\mathbf{x}, t) = \frac{\mu_0}{4\pi} \int d^3\mathbf{x}' \frac{1}{|\mathbf{x}-\mathbf{x}'|} j^\mu\left(\mathbf{x}', t - \frac{1}{c}|\mathbf{x}-\mathbf{x}'|\right). \quad (\text{J.81})$$

However, in one and two dimensions, the Liénard-Wiechert potentials sample charges and currents from the complete region inside the backward light cone,

$$A_{d=1}^\mu(x, t) = \frac{\mu_0 c}{2} \int_{-\infty}^{\infty} dx' \int_{-\infty}^{t-(|x-x'|/c)} dt' j^\mu(x', t'), \quad (\text{J.82})$$

$$A_{d=2}^\mu(\mathbf{x}, t) = \frac{\mu_0 c}{2\pi} \int d^2\mathbf{x}' \int_{-\infty}^{t-(|\mathbf{x}-\mathbf{x}'|/c)} dt' \frac{j^\mu(\mathbf{x}', t')}{\sqrt{c^2(t-t')^2 - (\mathbf{x}-\mathbf{x}')^2}}. \quad (\text{J.83})$$

Stated differently, a  $\delta$  function type charge-current fluctuation in the spacetime point  $x'$  generates an outwards traveling spherical electromagnetic perturbation on the forward light cone starting in  $x'$  if we are in three spatial dimensions. However, in one dimension the same kind of perturbation fills the whole forward light cone uniformly with electromagnetic fields, and in two dimensions the forward light cone is filled with a weight factor  $[c^2(t-t')^2 - (\mathbf{x}-\mathbf{x}')^2]^{-1/2}$ . How can that be? The electrostatic potentials (J.24) for  $d = 1$  and  $d = 2$  hold the answer to this. Those potentials indicate linear or logarithmic confinement of electric charges in low dimensions. Therefore a positive charge fluctuation in a point  $x'$  must be compensated by a corresponding negative charge fluctuation nearby. Both fluctuations fill their overlapping forward light cones with opposite electromagnetic fields, but those fields will exactly compensate in the overlapping parts in one dimension, and largely compensate in two dimensions. The net effect of these opposite charge fluctuations at a distance  $a$  is then electromagnetic fields along a forward light cone of thickness  $a$ , i.e. electromagnetic confinement in low dimensions effectively ensures again that electromagnetic fields propagate along light cones. This is illustrated in Figure J.1.



**Fig. J.1** The contributions of nearby opposite charge fluctuations at time  $t = 0$  in one spatial dimension generate net electromagnetic fields in the hatched "thick" light cone region

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