

↓ Lecture 14 [30.01.24]

16 | The BRT of electrodynamics:

Details: → Problemset 7

- i | Using  $\mathcal{L}_{\text{em}} = -\frac{1}{16\pi} F_{\mu\nu} F^{\mu\nu}$  and the transformation of a vector field (= spin-1)

$$\delta^{\alpha\beta} A_\mu = \frac{1}{2} \left( \delta_\mu^\alpha A^\beta - \delta_\mu^\beta A^\alpha \right) \quad (6.108)$$

in Eq. (6.102) yields the spin current:

$$S_{\text{em}}^{\mu\alpha\beta} \doteq \frac{1}{4\pi} \left( F^{\mu\alpha} A^\beta - F^{\mu\beta} A^\alpha \right) \quad (6.109)$$

- ii | Eq. (6.96) & Eq. (6.106) & Eq. (6.109) →

$$T_{\text{em}}^{\mu\nu} \doteq \frac{1}{4\pi} F^\mu_\rho F^{\rho\nu} - \eta^{\mu\nu} \mathcal{L}_{\text{em}} \quad (6.110a)$$

$$= \frac{1}{4\pi} \left[ F^\mu_\rho F^{\rho\nu} + \frac{\eta^{\mu\nu}}{4} F^{\rho\sigma} F_{\rho\sigma} \right] \quad (6.110b)$$

$$\doteq \left( \begin{array}{c|c} \mathcal{E} & c \vec{\Pi}^T \\ \hline c \vec{\Pi} & \Sigma \end{array} \right)_{\mu\nu} \quad (6.110c)$$

To show this you have to use the Maxwell equations in vacuum:  $\partial_\nu F^\nu_\mu = 0$ .

Components:

Energy density:  $\mathcal{E} = \frac{1}{8\pi} (\vec{E}^2 + \vec{B}^2) \quad (6.111a)$

Momentum density:  $\vec{\Pi} = \frac{1}{4\pi c} (\vec{E} \times \vec{B}) \quad (6.111b)$

\**Maxwell stress tensor*:  $\Sigma_{ij} = \frac{1}{4\pi} \left[ \frac{\delta_{ij}}{2} (\vec{E}^2 + \vec{B}^2) - E_i E_j - B_i B_j \right] \quad (6.111c)$

! Convince yourself that  $T_{\text{em}}^{\mu\nu}$  is *symmetric* and *gauge invariant*. Note that we did not construct it to be gauge invariant, only to be symmetric! We got this as a bonus.

- iii | The conservation  $\partial_\mu T^{\mu\nu} = 0$  of the BRT implies the following physical interpretations:
- $\nu = 0$ :

$$\partial_\mu T^{\mu 0} = \frac{1}{c} \frac{\partial \mathcal{E}}{\partial t} + c \nabla \cdot \vec{\Pi} = 0 \quad (6.112)$$

→ ↓ *Poynting's theorem* (in vacuum)

$$\frac{\partial \mathcal{E}}{\partial t} + \nabla \cdot \vec{S} = 0 \quad (6.113)$$

with

$$\Downarrow \text{Poynting vector: } \vec{S} = c^2 \vec{\Pi} = \frac{c}{4\pi} (\vec{E} \times \vec{B}) \quad (6.114)$$

Eq. (6.113) → Poynting vector = Energy current density

This is simply the formal statement of *energy conservation* for the free electromagnetic field. As energy is the Noether charge for translations in time, it is of course no coincidence that the Poynting theorem follows from the time-component  $\nu = 0$ .

- $\nu = i$ :

$$\partial_\mu T^{\mu i} = \frac{\partial \Pi_i}{\partial t} + \partial_k \Sigma_{ki} = 0 \quad (6.115)$$

→ Conservation of momentum with ...

- $\Pi_i$ :  $i$ -momentum density
- $\Sigma_{ki}$ :  $i$ -momentum current density

→ Maxwell stress tensor = Momentum current density

Note that are three momentum densities and corresponding current densities because there are three spatial momenta:  $i = x, y, z$ .

iv | Some final remarks:

- With the symmetric BRT one can define a gauge-invariant and conserved *angular momentum tensor*

$$M^{\rho\mu\nu} := T^{\rho\mu} x^\nu - T^{\rho\nu} x^\mu \quad (6.116)$$

with  $\partial_\rho M^{\rho\mu\nu} = 0$  (show this!). The conserved Noether charges are

$$J^{\mu\nu} := \frac{1}{c} \int d^3x M^{0\mu\nu} = \frac{1}{c} \int d^3x (T^{0\mu} x^\nu - T^{0\nu} x^\mu) \quad (6.117)$$

which encodes the *total angular momentum* of the field. Indeed, for the spatial components one finds

$$J_{ij} := \int d^3x (\Pi_i x_j - \Pi_j x_i) . \quad (6.118)$$

Since  $\Pi_i$  is the momentum density, the three components  $J_x \equiv J_{32}$ ,  $J_y \equiv J_{13}$  and  $J_z \equiv J_{21}$  can be identified as the total angular momentum  $\vec{J}$  of the field.

- If the electric current  $j^\mu$  does *not* vanish (i.e., the field is not in vacuum), the BRT derived above is no longer conserved. Rather one finds

$$\partial_\mu T_{\text{em}}^{\mu\nu} = -\frac{1}{c} F^{\nu\rho} j_\rho \quad (6.119)$$

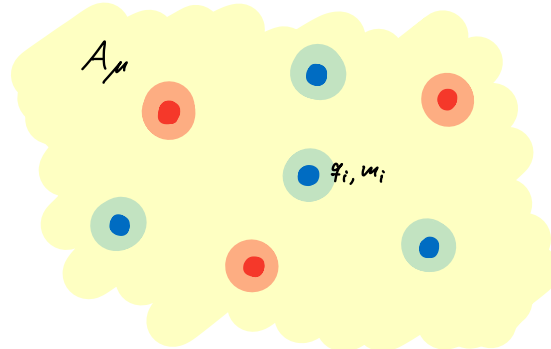
which can be identified as the *Lorentz force density*. This is perfectly reasonable as an external (non-dynamic) current  $j^\mu$  breaks the translation symmetry of the system in space and time on which the conservation of the BRT relies. Physically, the electromagnetic field is no longer a closed system because it can exchange momentum and energy with the charges described by  $j^\mu$ . Only if one describes the charges as dynamic degrees of freedom (→ *next section*) and considers the total BRT

$$T^{\mu\nu} = T_{\text{em}}^{\mu\nu} + T_{\text{charges}}^{\mu\nu} \quad (6.120)$$

one would recover the conservation  $\partial_\mu T^{\mu\nu} = 0$ ; this is then a statement about total energy and momentum conservation, including the energy and momentum of the charges.

## 6.4. Charged point particles in an electromagnetic field

1 |  $\llcorner$   $N$  charged point particles with charge  $q_i$  and mass  $m_i$  in a EM field  $A_\mu$ :



Eq. (6.56) & Eq. (5.41) → Relativistic action of the complete system:

$$S[\{x_k\}, A] = \int d^4x \left[ \underbrace{-\frac{1}{16\pi c} F_{\mu\nu} F^{\mu\nu}}_{\substack{S_{em}[A] \\ \text{EM field}}} - \underbrace{\frac{1}{c^2} A_\mu j^\mu}_{\substack{S_c[\{x_k\}, A] \\ \text{Coupling}}} \right] - \sum_{i=1}^N \underbrace{m_i c \int ds_i}_{\substack{S_p[x_i] \\ \text{Particle } i}} \quad (6.121)$$

$S_j[A]$ : EM field with static current  $j^\mu$

Note that the Lagrangian is a Lorentz scalar!  $S[\{x_k\}, A]$  is short for  $S[x_1, \dots, x_N, A]$ .  
with current density

$$j^\mu(x) \stackrel{6.18}{=} \sum_i \rho_i(x) \frac{dx_i^\mu}{dt} = \sum_i \underbrace{q_i \delta(\vec{x} - \vec{x}_i)}_{\text{Point particle}} \frac{dx_i^\mu}{dt}. \quad (6.122)$$

2 |  $\llcorner$  Coupling:

$$S_c[\{x_k\}, A] = -\frac{1}{c^2} \int d^4x A_\mu(x) j^\mu(x) \stackrel{\circ}{=} \sum_i \underbrace{\left\{ -\frac{q_i}{c} \int A_\mu(ct, \vec{x}_i) dx_i^\mu \right\}}_{S_c[x_i, A]} \quad (6.123)$$

Here we used  $\frac{dx_i^\mu}{dt} dt = dx_i^\mu$ ; the last integral is therefore a four-dimensional  $\downarrow$  *line integral* of the 4-vectorfield  $A_\mu$  along the trajectory of particle  $i$ .

3 | Hamilton's principle:

$$\delta S[x_k, A] = 0 \Leftrightarrow \begin{cases} \frac{\delta S_{em}[A]}{\delta A} + \frac{\delta S_c[\{x_k\}, A]}{\delta A} = \frac{\delta S_j[A]}{\delta A} = 0 \\ \forall_i : \frac{\delta S_c[x_i, A]}{\delta x_i} + \frac{\delta S_p[x_i]}{\delta x_i} = \frac{\delta S_A[\{x_k\}]}{\delta x_i} = 0 \end{cases} \quad (6.124)$$

**4 |** < Gauge field variations  $\delta A$ :

Here we don't have to do anything because we already computed the Euler-Lagrange equations:

$$\frac{\delta S_j[A]}{\delta A} = 0 \xleftrightarrow{6.56 \& 6.58} \partial_\nu F^{\nu\mu} \stackrel{6.122}{=} \frac{4\pi}{c} \sum_i q_i \delta(\vec{x} - \vec{x}_i) \frac{dx_i^\mu}{dt} \quad (6.125)$$

These are the inhomogeneous Maxwell equations with the  $N$  point particles as sources of the EM field. Note that this PDE system couples the particle coordinates  $\{x_k^\mu\}$  to the EM field  $A^\mu$ .

**5 |** < Particle trajectory variations  $\delta x_i$ :

i | Eqs. (6.121) and (6.123) →

$$S_A[\{x_k\}] = - \sum_i \int \left[ m_i c \sqrt{\dot{x}_{i\mu} \dot{x}_i^\mu} + \frac{q_i}{c} A_\mu(x_i) \dot{x}_i^\mu \right] d\lambda \quad (6.126)$$

Note that this action is again reparametrization invariant.

→ Euler-Lagrange equation for particle  $i$ :

$$\frac{\delta S_A[\{x_k\}]}{\delta x_i} = 0 \xleftrightarrow{x^\mu \equiv x_i^\mu} \frac{d}{d\lambda} \left[ \frac{m_i c \dot{x}_\mu}{\sqrt{\dot{x}_\mu \dot{x}^\mu}} \right] + \frac{q_i}{c} \left[ \dot{A}_\mu(x) - \dot{x}^\nu \frac{\partial A_\nu(x)}{\partial x^\mu} \right] = 0 \quad (6.127)$$

ii | Choose proper-time parametrization  $\lambda = \tau$ :

$$m_i \frac{du_\mu}{d\tau} + \frac{q_i}{c} \underbrace{\frac{dA_\mu}{d\tau}}_{\frac{\partial A_\mu}{\partial x^\nu} \frac{dx^\nu}{d\tau}} - \frac{\partial A_\nu}{\partial x^\mu} \frac{dx^\nu}{d\tau} = 0 \quad (6.128)$$

Thus we find as the EOM for particle  $i$ :

$$m_i \frac{du_\mu}{d\tau} = \frac{q_i}{c} \underbrace{\left( \frac{\partial A_\nu}{\partial x^\mu} - \frac{\partial A_\mu}{\partial x^\nu} \right)}_{F_{\mu\nu}} u^\nu \quad (6.129)$$

Or in the form discussed previously in Chapter 5 (we restore the particle index  $i$ ):

$$\frac{dp_i^\mu}{d\tau} = \frac{q_i}{c} F^\mu{}_\nu(x_i) u_i^\nu \quad (6.130)$$

with 4-momentum  $p_i^\mu = m_i u_i^\mu$ .

! The field strength tensor is evaluated at the position of the particle at a given time.

iii | Compare Eqs. (5.6) and (6.130) → 4-force:

$$K^\mu = \begin{pmatrix} \gamma_v \frac{\vec{F} \cdot \vec{v}}{c} \\ \gamma_v \vec{F} \end{pmatrix} = \frac{q_i}{c} F^\mu{}_\nu \gamma_v \frac{dx^\nu}{dt} \quad (6.131)$$

→ 3-force (we restore the particle index  $i$ ):

$$\vec{F}_i \stackrel{\circ}{=} q_i \vec{E}_i + \frac{q_i}{c} (\vec{v}_i \times \vec{B}_i) \quad \downarrow \text{Lorentz force} \quad (6.132)$$

with  $\vec{E}_i = \vec{E}(x_i)$ ,  $\vec{B}_i = \vec{B}(x_i)$  and  $\vec{v}_i = \frac{d\vec{x}_i}{dt}$ .

- This result demonstrates that our concept of the relativistic 3-force introduced in Eq. (5.11) was reasonable: for a force due to an electromagnetic field, it exactly matches the Lorentz force.
- It also demonstrates that the common expression for the Lorentz force is already fully relativistic. However, note that the 3-force determines the change rate of the *relativistic* 3-momentum  $\vec{p} = \gamma_v m \vec{v}$ , recall Eq. (5.16).

## 6 | Comments:

- Eqs. (6.125) and (6.130) together are the equations of motion of the composite system, i.e., the EM field and the  $N$  particles. Note that the system of differential equations is coupled: The dynamical positions of the particles determine the evolution of the EM field via Eq. (6.125), and the dynamical EM field determines the trajectories of the charged particles via Eq. (6.130).
- This model of  $N$  charged particles interacting with and via an electromagnetic field is the culmination of our discussion of *relativistic mechanics* in Chapter 5 and *electrodynamics* in Chapter 6.
- The theory Eqs. (6.125) and (6.130) is fully relativistic as the EOMs are manifestly Lorentz covariant (they are tensor equations).
- Note that this model describes interactions between the  $N$  particles not directly via forces (as one would in Newtonian mechanics), but via coupling to the dynamic EM field. Thus a particle can *locally* affect the EM field due to its motion, the EM field then can propagate with the speed of light through space and affect the trajectory of any other particle within the lightcone of the first. There is no instantaneous interaction between the particles!
- One can also consider the  $\mu = 0$  component of Eq. (6.130). Then one finds with  $p_i^0 = E_i/c$ :

$$\frac{dE_i}{dt} \stackrel{\circ}{=} q_i \vec{E}_i \cdot \vec{v}_i. \quad (6.133)$$

This is just the statement that the change of energy for particle  $i$  is given by the distance it travels collinear with the electric field per time. This is no surprise: The Lorentz force Eq. (6.132) tells us that the force due to the magnetic field is always perpendicular to the direction of motion and therefore cannot not perform work on the particle.

## 7 | Corollary: Single particle in a static electromagnetic field:

- i | The action follows from Eq. (6.126) with  $N = 1$  as:

$$S_A[x] = \int d\lambda L(x^\mu, \dot{x}^\mu) = - \int \left[ mc \sqrt{\dot{x}_\mu \dot{x}^\mu} + \frac{q}{c} A_\mu(x_i) \dot{x}^\mu \right] d\lambda \quad (6.134)$$

where  $A_\mu$  is a fixed parameter (the static field configuration).

- ii | < Parametrization in coordinate time  $\lambda = t$ :

$$L(\vec{x}, \vec{v}) = -mc^2 \sqrt{1 - \frac{v^2}{c^2}} + \frac{q}{c} \vec{A} \cdot \vec{v} - q \varphi \quad (6.135)$$

with  $A_\mu = (\varphi, -\vec{A})$  (covariant!) and  $\dot{\vec{x}} = \vec{v}$ .

iii | Canonical momentum:

$$\vec{\pi} := \frac{\partial L}{\partial \vec{v}} \stackrel{\circ}{=} m\gamma_v \vec{v} + \frac{q}{c} \vec{A} \quad (6.136)$$

with *mechanical momentum*  $\vec{p} = m\gamma_v \vec{v} \rightarrow$

$$\vec{p} = \vec{\pi} - \frac{q}{c} \vec{A} \quad (6.137)$$

$\vec{p}$ : Measurable momentum

→ Mechanical momentum  $\vec{p}$  gauge-invariant

→ Canonical momentum  $\vec{\pi}$  *not* gauge-invariant

iv | Hamiltonian:

$$H = \vec{\pi} \cdot \vec{v} - L \stackrel{\circ}{=} \underbrace{\frac{mc^2}{\sqrt{1 - \frac{v^2}{c^2}}}}_{E} + q\varphi \stackrel{5.26}{=} c \sqrt{\left(\pi - \frac{q}{c} \vec{A}\right)^2 + m^2 c^2} + q\varphi \quad (6.138)$$

so that

$$E = H - q\varphi \quad (6.139)$$

$E$  is gauge invariant →  $H$  is *not* gauge invariant

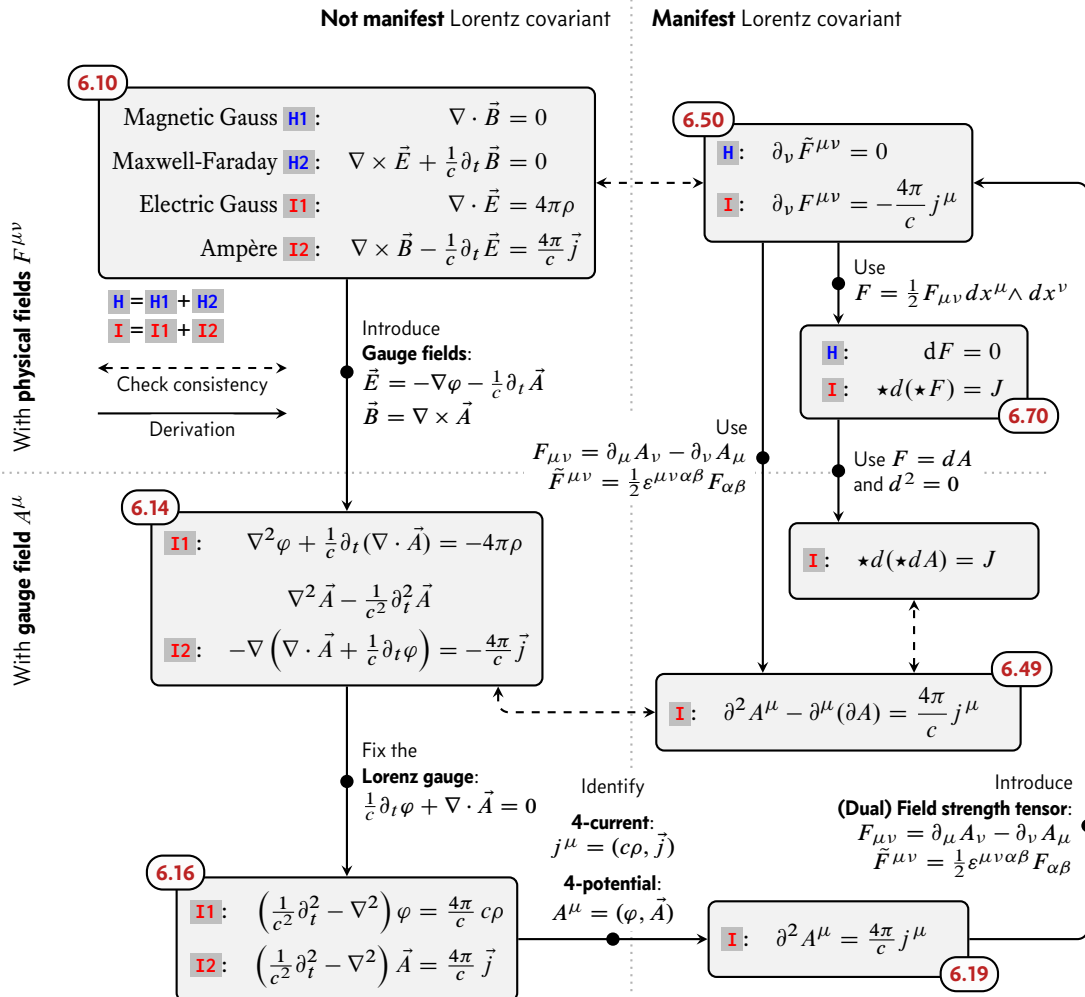
v | Summary:

$$\text{Gauge invariant} \left\{ \begin{array}{l} E = H - q\varphi \\ \vec{p} = \vec{\pi} - \frac{q}{c} \vec{A} \end{array} \right\} \Leftrightarrow \left\{ \begin{array}{l} E + q\varphi = H \\ \vec{p} + \frac{q}{c} \vec{A} = \vec{\pi} \end{array} \right\} \text{Gauge dependent} \quad (6.140)$$

For more details on the aspect of the gauge-(in)variance of certain quantities, see Ref. [79]. Note that these subtleties are not specific to a relativistic treatment, they already appear in Newtonian mechanics (only the specific dependency of the Hamiltonian on the mechanical/canonical momentum and the functional form of the Lagrangian are relativistic).

### 6.5. Summary: The many faces of Maxwell's equations

Here is a compact overview over the many (physically equivalent) forms of Maxwell's equations that we encountered in this chapter:



## 7. Relativistic Field Theories II: Relativistic Quantum Mechanics

### Reminder

- 1 | The ↓ *Schrödinger equation* (SE)

$$i\hbar\partial_t\psi(t, \vec{x}) = \hat{H}\psi(t, \vec{x}) \quad (7.1)$$

is a linear field equation with ↓ *Hamilton operator*

$$\hat{H} = \frac{\vec{p}^2}{2m} + V(\vec{x}) = -\frac{\hbar^2}{2m}\Delta + V(\vec{x}) \quad (7.2)$$

and the complex-valued field  $\psi : \mathbb{R}^{1,3} \rightarrow \mathbb{C}$ .

It describes the time evolution of a single quantum particle with mass  $m$  in a potential  $V(\vec{x})$  that is initially described by the wavefunction  $\psi_0(\vec{x}) = \psi(0, \vec{x})$  at  $t = 0$ .

- 2 | The wavefunction has the interpretation

$$|\psi(t, \vec{x})|^2 = \langle \text{Probability to find particle at time } t \text{ at position } \vec{x} \rangle \quad (7.3)$$

which necessitates the normalization condition

$$\forall_t : \quad \|\psi(t)\|_2 := \int d^3x |\psi(t, \vec{x})|^2 = 1. \quad (7.4)$$

Thus the wavefunction is an element of the Hilbert space  $\psi \in L^2 \equiv L^2(\mathbb{R}^3, \mathbb{C})$  of square-integrable functions.

The Hermiticity  $\hat{H} = \hat{H}^\dagger$  of the Hamiltonian implies a unitary time evolution and thereby guarantees a conserved norm:

$$\frac{d}{dt}\|\psi(t)\|_2 = \int d^3x [\psi^* \partial_t \psi + \psi \partial_t \psi^*] \stackrel{7.1}{=} \frac{1}{i\hbar} \int d^3x [\psi^* (\hat{H}\psi) - \psi (\hat{H}\psi)^*] \stackrel{7.6}{=} 0, \quad (7.5)$$

where we used that for  $\psi, \phi \in L^2$  and a Hermitian Hamiltonian

$$\int d^3x \phi^* (\hat{H}\psi) \stackrel{\text{def}}{=} \langle \phi | \hat{H} \psi \rangle \stackrel{\text{def}}{=} \langle \hat{H}^\dagger \phi | \psi \rangle \stackrel{\text{def}}{=} \int d^3x (\hat{H}^\dagger \phi)^* \psi \stackrel{\hat{H}=\hat{H}^\dagger}{=} \int d^3x \psi (\hat{H}\phi)^*. \quad (7.6)$$

- 3 | Problem: The SE is Galilei covariant but *not* Lorentz covariant! (recall ↻ Problemset 1)

- The SE is of first order in time but of second order in the spatial derivatives. This asymmetry already suggests that the equation cannot be Lorentz covariant: Time is treated differently than space in (non-relativistic) quantum mechanics.
- We would like quantum mechanics to be described by a Lorentz covariant equation because we subscribed to ← *Einstein's principle of special relativity* **SR** at the beginning of this course: All laws of physics must take the same form in all inertial systems (which are related by Lorentz transformations). This certainly includes quantum mechanics.

However, **SR** is just a (empirically motivated) *principle*, it is neither a law nor a theorem; there may be conceivable universes in which **SR** simply does not apply to the quantum realm – in which case the Schrödinger Eq. (7.1) would be a perfectly valid model.

As good physicists, we should seek for empirical evidence to settle the matter ...



4 | Evidence:

- First: The Schrödinger equation, published and studied by Erwin Schrödinger in a sequence of papers in 1926 [80–83] (so RELATIVITY was already known at the time), was (and is) a highly successful theory that describes a plethora of microscopic phenomena remarkably well. Examples are the ↓ *double-slit experiment*, ↓ *quantum tunneling effects*, and, of course, the ↓ *spectrum of the hydrogen atom*:

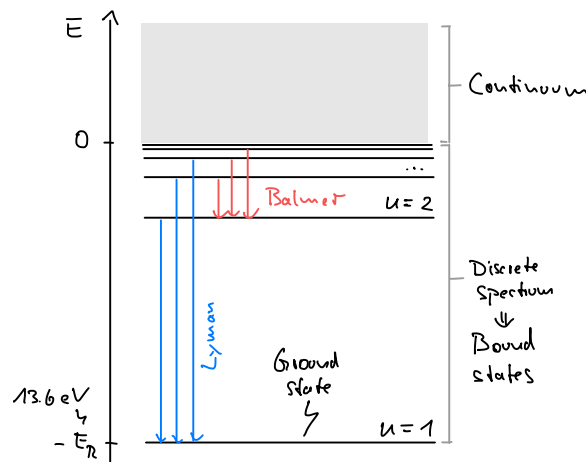
The Hamilton operator for the relative electron-proton system of the hydrogen atom is

$$\hat{H} = -\frac{\hbar^2}{2\mu} \nabla^2 - \frac{e^2}{|\vec{x}|} \tag{7.7}$$

with reduced mass  $\mu = m_e m_p / (m_e + m_p)$ . The discrete part of the spectrum of the operator  $\hat{H}$  can be computed exactly ( $E_R$  is the ↓ *Rydberg energy*),

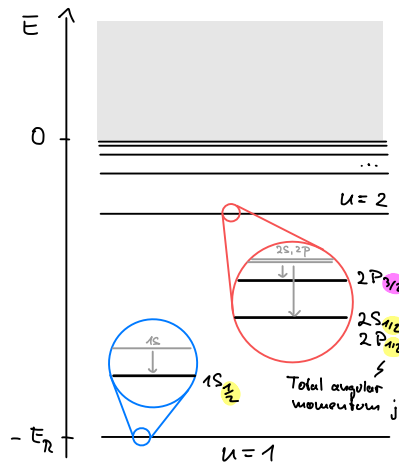
$$E_n = -\frac{E_R}{n^2} \quad \text{with principal quantum number } n \in \{1, 2, \dots\}, \tag{7.8}$$

and determines the hydrogen spectrum:



The transitions between the levels of the hydrogen spectrum can be measured by spectroscopy (↓ *Lyman series* [84], ↓ *Balmer series* [85], ...; these observations have been made around 1900). The explanation of these spectral lines by the non-relativistic Schrödinger equation is the crown jewel of quantum mechanics, and one of the most remarkable advances of 20th century physics.

- However, it’s not all sunshine and roses. It was already known at the end of the 19th century (due to advances in spectroscopy [86]) that the spectral lines of various atomic species (including hydrogen) had a ↓ *fine-structure*. Expressed in terms of the energy levels of the hydrogen atom, this means that some of the degenerate eigenstates of Eq. (7.7) are actually *not exactly* degenerate:



Note that this was known to Schrödinger when he published his equation in 1926; he writes in Ref. [83] (p. 132–133):

*Im Anschluß an die zuletzt erwähnten physikalischen Probleme, [..], möchte ich nun doch die vermutliche relativistisch-magnetische Verallgemeinerung der Grundgleichungen [..] hier ganz kurz mitteilen, wenn ich es auch vorerst nur für das Einelektronenproblem und nur mit der allergrößten Reserve tun kann. Letzteres aus zwei Gründen. Erstens beruht die Verallgemeinerung vorläufig auf rein formaler Analogie. Zweitens führt sie, wie schon in der ersten Mitteilung erwähnt wurde, im Falle des Keplerproblems zwar formal auf die Sommerfeldsche Feinstrukturformel und zwar mit „halbzahligen“ Azimutal- und Radialquant, was heute allgemein als korrekt angesehen wird; allein es fehlt noch die zur Herstellung numerisch richtiger Aufspaltungsbilder der Wasserstofflinien notwendige Ergänzung, die im Bohrschen Bilde durch den Goudsmit-Uhlenbeck'schen Elektronendrehimpuls geliefert wird.*

Note that Schrödinger was very much aware that his equation lacked Lorentz covariance and viewed (and constructed) it as a *non-relativistic approximation* of a truly “relativistic quantum mechanics” (which he didn’t know how to formulate consistently).

He also makes this clear in the introduction of Ref. [82] (p. 439):

*Wesentlich größeres Interesse wird natürlich die (hier noch nicht durchgeführte) Anwendung auf den Zeemaneffekt bieten. Diese erscheint mir unlöslich geknüpft an eine korrekte Formulierung des relativistischen Problems in der Sprache der Wellenmechanik, weil bei vierdimensionaler Formulierung das Vektorpotential von selbst dem skalaren ebenbürtig an die Seite tritt. Schon in der ersten Mitteilung wurde erwähnt, daß das relativistische Wasserstoffatom sich zwar ohne weiteres behandeln läßt, aber zu „halbzahligen“ Azimutalquanten, also zu einem Widerspruch mit der Erfahrung führt. Es mußte also noch „etwas fehlen“. Seither habe ich [..] gelernt, was fehlt: in der Sprache der Elektronenbahentheorie der Drehimpuls des Elektrons um seine Achse, der ihm ein magnetisches Moment verleiht.*

- We can also make a back-of-the-envelope calculation to estimate whether relativistic effects could be the root cause for the discrepancy between the non-relativistic Schrödinger equation and the observed fine-structure:

In a *classical* approximation, kinetic and potential energy are of the same order:

$$\text{Kinetic energy } \frac{1}{2}mv^2 \sim \frac{e^2}{r} \quad \text{Potential energy} . \quad (7.9)$$

Because the system is quantum, momentum and position obey the  $\downarrow$  *Heisenberg uncertainty relation*  $\Delta p \Delta r \sim \hbar$ . In the energy eigenstates of an interacting quantum system (like an atom) we typically have  $\Delta p \sim p$  and  $\Delta r \sim r$ , and in our semi-classical approximation it is

$p \sim mv$ , so that

$$v \sim \frac{e^2}{mvr} \sim \frac{e^2}{\hbar c} = \alpha c = \text{Fine-structure constant} \times c \approx \frac{c}{137}. \quad (7.10)$$

The semi-classical velocity of the electron  $v$  is therefore much smaller than the speed of light  $c$ ; this explains why the non-relativistic Schrödinger equation is so successful (and your course non-relativistic quantum mechanics is no waste of time). However, the observed fine-structure splitting of spectral lines is indeed very small, so it is reasonable that relativistic effects can have small but measurable effects in atomic physics.

The situation is therefore similar to that of Newtonian mechanics before we made it relativistic: We have a very successful Galilei covariant theory that, however, shows signs of being the low-velocity/energy approximation of another, presumably relativistic theory.

(Note that *historically* the situation is very different, though: While Newtonian mechanics, born in the 17th century, had to wait more than 200 years to be “made relativistic”, the development of relativistic quantum mechanics was very fast: Non-relativistic quantum mechanics was established in 1925/26 – and just two years later, in 1928, Paul Dirac published the correct equation describing relativistic electrons: the → *Dirac equation* [87].)

→ Are there relativistic field equations which allow for a probabilistic interpretation?

## 7.1. The Klein-Gordon equation

The Klein-Gordon equation has been studied by Klein [88] and Gordon [89] in 1926 as a possible relativistic version of the Schrödinger equation. Schrödinger and Fock found the equation independently as well.

1 |  $\triangleleft$  *Complex* scalar field:  $\phi : \mathbb{R}^{1,3} \rightarrow \mathbb{C}$

→ Most general *quadratic* (superposition principle!) and *Lorentz covariant* Lagrangian density:

$$\mathcal{L}_{\text{KG}}(\phi, \partial\phi) = (\partial^\mu \phi)(\partial_\mu \phi^*) - M^2 \phi \phi^* \quad (7.11)$$

$M = \frac{mc}{\hbar} \in \mathbb{R}$ : arbitrary parameter ( $m$  will be the mass of the particle)

- Note that  $M = \frac{mc}{\hbar} = \frac{2\pi}{\lambda}$  has the dimension of an inverse length; here  $\lambda = \frac{h}{mc}$  is the  $\triangleleft$  *Compton wavelength* Eq. (5.77).
- One can also derive the non-relativistic Schrödinger equation from a Lagrangian density (→ below):

$$\mathcal{L}_{\text{SE}}(\psi, \partial\psi) = i\hbar\psi^* \partial_t \psi - \frac{\hbar^2}{2m} (\nabla\psi^*)(\nabla\psi) - V(x)\psi^* \psi \quad (7.12)$$

This is of course not a Lorentz scalar (you cannot write this combining only tensors).

2 | Euler-Lagrange equations:

*Trick:* Consider  $\phi$  and  $\phi^*$  as *independent* fields; let  $\phi^*$  be the complex conjugate of  $\phi$  at the end.

$$\frac{\partial \mathcal{L}_{\text{KG}}}{\partial \phi^*} - \partial_\mu \frac{\partial \mathcal{L}_{\text{KG}}}{\partial (\partial_\mu \phi^*)} = 0 \quad \Rightarrow \quad -M^2 \phi - \partial_\mu \partial^\mu \phi = 0 \quad (7.13)$$

The Euler-Lagrange equations for the field  $\phi$  yield the complex conjugate Klein-Gordon equation.

→

$$(\partial^2 + M^2)\phi(x) = 0 \quad \text{** Klein-Gordon equation} \quad (7.14)$$

The Klein-Gordon equation (KGE) is the simplest relativistic wave equation.

The non-relativistic Schrödinger equation follows along the same lines from Eq. (7.12):

$$\frac{\partial \mathcal{L}_{SE}}{\partial \psi^*} - \partial_\mu \frac{\partial \mathcal{L}_{SE}}{\partial (\partial_\mu \psi^*)} = 0 \quad \Rightarrow \quad i \hbar \partial_t \psi - V \psi + \frac{\hbar^2}{2m} \nabla^2 \psi = 0 \quad (7.15)$$

The Euler-Lagrange equations for  $\psi^*$  yield the complex conjugate of the Schrödinger equation.

### 3 | Lorentz symmetry of the KGE:

The KGE is manifest Lorentz covariant. However, it is instructive (and useful for our derivation of the Dirac equation → later) to check its invariance manually. To this end, we view Lorentz transformations as *active* transformations, mapping solutions to different solutions. This is equivalent to the *passive* viewpoint where the coordinate system is transformed instead:

i |  $\triangleleft$  Coordinate transformation:  $\bar{x} = \Lambda x$  & Field transformation:  $\bar{\phi}(\bar{x}) = \phi(x)$   
We write  $\bar{x} = \Lambda x$  for  $\bar{x}^\mu = \Lambda^\mu_\nu x^\nu$ .

ii |  $\triangleleft \phi(x)$  with  $(\partial^2 + M^2)\phi(x) = 0$  for all  $x$   
That is,  $\phi(x)$  is a solution of the KGE.

iii |  $\xrightarrow{\circ} \bar{\phi}(x) := \phi(\Lambda^{-1}x)$  is a *new solution*:

Use the chain rule in the first step twice:

$$(\eta^{\mu\nu} \partial_\mu \partial_\nu + M^2)\bar{\phi}(x) = [\eta^{\mu\nu} (\Lambda^{-1})^\sigma_\mu \partial_\sigma (\Lambda^{-1})^\rho_\nu \partial_\rho + M^2]\phi(\Lambda^{-1}x) \quad (7.16a)$$

$$\text{Use invariance of the metric Eq. (4.21)} \quad (7.16b)$$

$$= (\eta^{\sigma\rho} \partial_\sigma \partial_\rho + M^2)\phi(\Lambda^{-1}x) \quad (7.16c)$$

$$= (\partial^2 + M^2)\phi(\Lambda^{-1}x) \stackrel{\phi \text{ solution}}{=} 0 \quad (7.16d)$$

Here  $\partial_\sigma \phi(\Lambda^{-1}x)$  must be read as  $\partial_\sigma \phi(y)|_{y=\Lambda^{-1}x}$ , i.e., we compute the derivative of the function  $\phi$  with respect to its argument  $y$  and then plug in the value  $\Lambda^{-1}x$ .

### 4 | Conserved current:

i |  $\triangleleft$  Global phase rotations:

$$\phi'(x) = e^{i\alpha} \phi(x) \quad \text{for } \alpha \in [0, 2\pi) \quad (7.17)$$

with infinitesimal generator  $|\alpha| = |w| \ll 1$

$$\phi'(x) = \phi(x) + iw\phi(x) \equiv \phi(x) + w \delta\phi(x) \quad \Rightarrow \quad \delta\phi = i\phi \quad (7.18)$$

Note that this is an “internal symmetry” that has nothing to do with spacetime; thus  $\delta x = 0$ . For the complex conjugate field  $\phi^*$  one finds analogously  $\delta\phi^* = -i\phi^*$ .

→ Continuous symmetry:

$$\mathcal{L}_{KG}(\phi, \partial\phi) = \mathcal{L}_{KG}(\phi', \partial\phi') \quad (7.19)$$

If the Lagrangian density is invariant, the action is trivially invariant!

ii | Noether theorem Eq. (6.85) → Conserved Noether current density Eq. (6.84):

$$j_{\text{KG}}^\mu \stackrel{\circ}{=} i(\partial^\mu \phi)\phi^* - i(\partial^\mu \phi^*)\phi \quad (7.20)$$

Note that if one treats  $\phi$  and  $\phi^*$  independent fields, one has to sum over the two fields in the evaluation of the Noether current; this then yields the real-valued current density above.

→ Noether charge density:

$$\rho_{\text{KG}}(x) := j_{\text{KG}}^0(x) = \frac{i}{c} (\dot{\phi}\phi^* - \dot{\phi}^*\phi) \quad \text{with} \quad \rho_{\text{KG}}(x) \in \mathbb{R} \quad (7.21)$$

→ Conserved Noether charge:

$$Q = \int d^3x \rho_{\text{KG}}(x) = \frac{i}{c} \int d^3x (\dot{\phi}\phi^* - \dot{\phi}^*\phi) \quad (7.22)$$

Important:  $\rho_{\text{KG}}(x) \not\geq 0$  is *not* positive-definit! →

$$\rho_{\text{KG}}(x) \text{ cannot be interpreted as a probability density!} \quad (7.23)$$

• To sum up:

- The inner product (= positive-definite, symmetric sesquilinear form) on  $L^2(\mathbb{R}^{1,3}, \mathbb{C})$

$$\langle \phi | \psi \rangle_{L^2} := \int d^3x \phi^* \psi \quad (7.24)$$

is *not* conserved under the time-evolution of the KGE.

- The *indefinite* symmetric sesquilinear form (which is not an inner product!)

$$\langle \phi | \psi \rangle_{\text{KG}} := \frac{i\hbar}{2mc^2} \int d^3x (\phi^* \dot{\psi} - \dot{\phi}^* \psi) \quad (7.25)$$

is conserved under the time-evolution of the KGE. But because it is not positive-(semi)definite, we cannot interpret the induced “norm” as a probability.

The prefactor  $\frac{\hbar}{2mc^2}$  is chosen such that it has the dimension of a time (because  $\frac{\hbar}{mc} \propto \lambda$  has the dimension of a length). Then the square of the fields (= wavefunctions) has the dimension of one over a volume – which is the conventional dimension of wavefunctions. The factor  $\frac{1}{2}$  is chosen to simplify expressions later.

- Compare this to the conserved current for the same phase rotation symmetry that follows for the Schrödinger field Eq. (7.12) with  $\delta\psi = i\psi$  and  $\delta\psi^* = -i\psi^*$ :

$$j_{\text{SE}}^\mu \equiv \begin{pmatrix} \hbar c \rho_{\text{SE}} \\ \hbar \vec{j}_{\text{SE}} \end{pmatrix} \stackrel{7.12}{\stackrel{6.84}{=}} \begin{cases} \hbar c \psi^* \psi, & \mu = 0 \\ \frac{i\hbar^2}{2m} [(\nabla\psi^*)\psi - (\nabla\psi)\psi^*] & \mu = i = 1, 2, 3 \end{cases} \quad (7.26)$$

(Recall that you must sum over the fields  $\psi$  and  $\psi^*$ .)

This is the *positive-definite probability density* you already know from quantum mechanics,

$$\rho_{\text{SE}}(x) = \psi^*(x)\psi(x) = |\psi(x)|^2 \geq 0, \quad (7.27)$$

and the ↓ *probability current density*

$$\vec{j}_{SE} = \frac{i\hbar}{2m} [(\nabla\psi^*)\psi - (\nabla\psi)\psi^*]. \quad (7.28)$$

In this context, Noether's theorem ensures probability conservation:

$$\partial_\mu j_{SE}^\mu = 0 \quad \Leftrightarrow \quad \partial_t \rho_{SE} + \nabla \cdot \vec{j}_{SE} = 0. \quad (7.29)$$

## 5 | Solutions: (for the free Klein-Gordon field)

i | The KG Eq. (7.14) is a wave equation:

$$\left[ \frac{1}{c^2} \partial_t^2 - \nabla^2 + \frac{m^2 c^2}{\hbar^2} \right] \phi(t, \vec{x}) = 0 \quad (7.30)$$

→ Solution space spanned by plane waves:

$$\phi(t, \vec{x}) = e^{\frac{i}{\hbar}(\vec{p} \cdot \vec{x} - Et)} \quad (7.31)$$

Plug this ansatz into Eq. (7.30) → Dispersion relation:

$$-\frac{E^2}{c^2 \hbar^2} + \frac{\vec{p}^2}{\hbar^2} + \frac{m^2 c^2}{\hbar^2} \stackrel{!}{=} 0 \quad (7.32)$$

$$E = \pm \sqrt{\vec{p}^2 c^2 + m^2 c^4} \quad (7.33)$$

- This is the relativistic energy-momentum relation Eq. (5.26).
  - ¡! There are *two* solutions for each 3-momentum  $\vec{p}$ , one of which has *negative* energy  $E < 0$  (if we interpret the prefactor of  $t$  as the energy as usual). This is a consequence of the quadratic nature of the KGE (as compared to the SE), and therefore a direct consequence of its relativistic covariance.
  - At the time of its inception, the negative energy solutions of the KGE could not be interpreted properly. This (together with the fact that its conserved “norm” cannot be interpreted as a probability and it fails to predict the fine-structure of the hydrogen atom correctly, → *below*) lead to its dismissal as a relativistic wave equation for quantum wave functions. It only became clear later that the negative energy solutions herald the existence of *antiparticles*. Only in modern ↑ *relativistic quantum field theories* [where the KGE reappears as the equation of motion of (free scalar) quantum fields, see Chapter 2 of my script on QFT [19]] this “feature” can be cast into a consistent framework: The negative energy solutions are interpreted as eigenmodes of antiparticles with *positive* energies (and norms). If the particles are charged, their antiparticles have opposite charge; then the conserved Noether charge Eq. (7.22) is interpreted as *charge conservation* (and not probability conservation).
- ii | As usual, one can “normalize” the plane wave solutions Eq. (7.31) if one considers a finite system with volume  $V = L^3$ . Then one finds the “orthonormal” solution basis of the KGE:

→

$$\phi_{\vec{k}}^{(\pm)}(t, \vec{x}) = N_{\vec{k}} e^{i(\vec{k} \cdot \vec{x} \mp \omega_k t)} \quad \text{with ...} \quad (7.34a)$$

$$\text{Dispersion:} \quad \omega_k = \sqrt{\vec{k}^2 c^2 + m^2 c^4 / \hbar^2}$$

$$\text{Momentum:} \quad \vec{p} = \hbar \vec{k} \in \hbar \frac{2\pi}{L} \mathbb{Z}^3 \quad (7.34b)$$

$$\text{Normalization:} \quad N_k = \sqrt{\frac{mc^2}{V \hbar \omega_k}}$$

- It is straightforward to check that these states are “orthonormal” with respect to the Klein-Gordon sesquilinear form Eq. (7.25):

$$\langle \psi_{\vec{k}}^{(\alpha)} | \psi_{\vec{k}'}^{(\beta)} \rangle_{\text{KG}} \stackrel{\circ}{=} \alpha \delta_{\alpha, \beta} \delta_{\vec{k}, \vec{k}'} \quad \text{with} \quad \alpha, \beta \in \{\pm\}. \quad (7.35)$$

Note that the (−) states have negative “norm”.

- The fact that there are “twice as many” linearly independent solutions (two for each momentum) means that you need “twice as many” parameters to specify a particular solution (i.e., a linear combination of the plane waves). This corresponds to the fact that the KGE is of *second order* in the time derivative, so that you need to provide both  $\phi(t = 0, \vec{x})$  and  $\dot{\phi}(t = 0, \vec{x})$  to specify a unique solution.