6 Klein-Gordon equation

6.1 Basics of special relativity

The Schrödinger equation is a non-relativistic equation. That means that it is form-invariant under Galilei transformations. Observables predicted by the Schrödinger equation, provided they are scalars, obtain the same value in any coordinate system related by Galilei transformations.

However, we know that Galilei symmetry is not the correct symmetry of nature. It holds only approximately for coordinate systems (or system components) moving relative to each other at small velocity, i.e., significantly smaller than the speed of light.

The true symmetry of the laws of nature (in flat space) is Poincaré symmetry. Poincaré transformations are the set of linear transformations of spacetime coordinates

$$x^\mu = (x^0, x^1, x^2, x^3) \equiv (ct, x^1, x^2, x^3) \qquad (6.1)$$

of the form

$$x'^\mu = \Lambda^\mu{}_\nu x^\nu + a^\mu , \qquad (6.2)$$

that leave the bilinear form build out of two vectors ξ^μ, η^μ (in the tangent space at x^μ)

$$(\xi, \eta) = \xi^0 \eta^0 - \xi^1 \eta^1 - \xi^2 \eta^2 - \xi^3 \eta^3 \tag{6.3}$$

$$= g_{\mu\nu} \xi^\mu \eta^\nu$$

with the metric

$$g_{\mu\nu} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \tag{6.4}$$

invariant. For two space time points x^μ and y^μ, this bilinear form defines an invariant distance:

$$d(x, y) = g_{\mu\nu} (x-y)^\mu (x-y)^\nu . \tag{6.5}$$

It is convenient to introduce so-called covariant vectors with lower indices (in contradistinction to contra-variant vectors with upper indices):

$$\xi_\mu := g_{\mu\nu} \xi^\nu$$

such that $(\xi, \eta) = g_{\mu\nu} \xi^\mu \eta^\nu = \xi^\mu \eta_\mu = \xi_\mu \eta^\mu$ (6.6)

The metric is obviously identical to its own inverse $\quad g_{\mu\nu} = g^{\mu\nu}$, such that

$$g_{\mu\nu}\, g^{\nu\kappa} = \delta_\mu^\kappa \tag{6.7}$$

The 4-vector a^μ in (6.2) obviously parameterizes constant shifts in spacetime. As it drops out in coordinate differences:

$$(x'-y')^\mu = \Lambda^\mu{}_\nu\, (x-y)^\nu, \tag{6.8}$$

the invariance of distances implies

$$g_{\mu\nu} = g_{\kappa\lambda}\, \Lambda^\kappa{}_\mu\, \Lambda^\lambda{}_\nu \tag{6.9}$$

Matrices $\Lambda^\mu{}_\nu$ that obey (6.9) define the set of Lorentz transformations.

3d space rotations form a subset of Lorentz transformations, given by

$$\Lambda = \begin{pmatrix} 1 & 0 \\ 0 & R \end{pmatrix}, \quad R \in SO(3) \tag{6.10}$$

Further transformations are related to

Lorentz boosts, i.e., transformations between different coordinate frames moving relatively to each other at constant speed $\vec{v}$.

For instance if $\vec{v} = v \cdot \hat{e}_1$, the corresponding $\Lambda^\mu{}_\nu$ is given by

$$\Lambda = \begin{pmatrix} \gamma & \gamma\beta & 0 & 0 \\ \gamma\beta & \gamma & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \tag{6.11}$$

reproducing the well-known 1D Lorentz transformations

$$\begin{aligned} x'^0 &= \gamma(x^0 + \beta x^1) \\ x'^1 &= \gamma(\beta x^0 + x^1) \\ x'^2 &= x^2, \quad x'^3 = x^3 . \end{aligned} \qquad , \quad \beta = \frac{v}{c} \tag{6.12}$$

In total, Lorentz transformations constitute a 6-parameter family of transformations:

3 boost parameters (e.g. a velocity 3-vector) (6.13)

3 rotation parameters (e.g. 3 Euler angles).

6.2 Klein-Gordon equation

Schrödinger, of course, knew about the requirement of Poincaré or Lorentz invariance of fundamental physical laws. What is now known as Klein-Gordon equation was actually Schrödinger's first attempt at constructing a wave equation for quantum particles. However, he realized that the relativistic equation didn't predict the fine-structure correctly and then turned to the non-relativistic limit.

The non-relativistic Schrödinger equation can be inferred from the non-relativistic energy momentum relation

$$E = \frac{\vec{p}^{\,2}}{2m} \qquad (6.14)$$

by using the correspondence rule

$$E \to -\frac{\hbar}{i}\partial_t \quad \text{and} \quad \vec{p} \to \frac{\hbar}{i}\vec{\nabla}. \qquad (6.15)$$

This correspondence may be motivated by

the requirement that a free particle is described by a plane wave

$$\psi(t,\vec{x}) = e^{\frac{i}{\hbar}(\vec{p}\,\vec{x} - Et)} \tag{6.16}$$

$$\Rightarrow \quad i\hbar\,\partial_t \psi = \frac{1}{2m}\left(\frac{\hbar}{i}\vec{\nabla}\right)^2 \psi$$

Along the same line of reasoning, we consider the relativistic energy-momentum relation:

$$E^2 = \vec{p}^{\,2} c^2 + (mc^2)^2 . \tag{6.17}$$

Introducing the 4-momentum

$$p^\mu = \begin{pmatrix} E/c \\ \vec{p} \end{pmatrix}, \quad p_\mu = \begin{pmatrix} E/c \\ -\vec{p} \end{pmatrix}, \tag{6.18}$$

this can be written as

$$(p,p) = p^\mu p_\mu = m^2 c^2 \tag{6.19}$$

The correspondence rule $\overset{(6.15)}{}$ in 4-notation can be summarized as

$$p_\mu \rightarrow i\hbar\,\partial_\mu \equiv i\hbar \frac{\partial}{\partial x^\mu} \tag{6.20}$$

The wave equation resulting from (6.19) or (6.17) then is

$$\left(\Box + \frac{m^2 c^2}{\hbar^2} \right) \phi(x) = \left(\Box + \mu^2 \right) \phi(x) = 0 \tag{6.21}$$

Klein-Gordon equation

Here,

$$\Box = \frac{\partial^2}{\partial (ct)^2} - \vec{\nabla}^2 = \partial_\mu \partial^\mu \tag{6.22}$$

is the D'Alembert operator, and

$$\mu = \frac{mc}{\hbar} \tag{6.23}$$

is the inverse Compton wave length of a particle of mass m.

It is easy to check that the Klein-Gordon equation is Lorentz invariant, as ∂_μ transforms as a (covariant) 4-vector,

$$\partial_\mu = \frac{\partial}{\partial x^\mu} = \frac{\partial x'^\kappa}{\partial x^\mu} \frac{\partial}{\partial x'^\kappa} = \Lambda^\kappa{}_\mu \, \partial'_\kappa \tag{6.24}$$

and thus

$$\begin{aligned} \Box = \partial_\mu \partial_\nu g^{\mu\nu} &= \partial'_\kappa \partial'_\lambda \Lambda^\kappa{}_\mu \Lambda^\lambda{}_\nu \, g^{\mu\nu} \\ &= \partial'_\kappa \partial'_\lambda \, g^{\kappa\lambda} = \Box' \end{aligned} \tag{6.25}$$

Hence, if $\phi(x)$ satisfies the Klein-Gordon equation in one inertial frame, $\phi'(x') = \phi(x)$ satisfies the Klein-Gordon equation in the inertial frame defined by the coordinates x'.

Probability interpretation

A crucial aspect of nonrelativistic QM is the interpretation of the wave function as a probability amplitude. The associated conservation of probability in a unitary time evolution is encoded in the continuity equation relating the probability density $\rho = \psi^* \psi$ and the probability current $\vec{j} \sim \operatorname{Im} \psi^* \vec{\nabla} \psi$,

$$\partial_t \rho + \vec{\nabla} \cdot \vec{j} = 0 . \qquad (6.26)$$

Let us check whether similar quantities exist for the Klein-Gordon equation. For this, we note that also the complex conjugate wave function satisfies the Klein-Gordon equation,

$$(\Box + \mu^2)\, \phi^* = 0$$

$$\Rightarrow \quad \phi^* \Box \phi - \phi \Box \phi^* = -\mu^2 (\phi^* \phi - \phi \phi^*) = 0 \qquad (6.27)$$

The left-hand side implies

$$\partial_\mu \left(\varphi^* \partial^\mu \varphi - \varphi \, \partial^\mu \varphi^* \right) = 0 \,, \qquad (6.28)$$

such that the covariant current density

$$j^\mu = \frac{i\hbar}{2m} \left(\varphi^* \partial^\mu \varphi - \varphi \partial^\mu \varphi^* \right) \qquad (6.29)$$

is conserved for any solution of the Klein-Gordon equation,

$$\partial_\mu j^\mu = 0 \,. \qquad (6.30)$$

This current is identical to the Noether current of the symmetry of the Klein-Gordon equation under global phase transformations. Since

$$\partial_0 \int d^3x \; j^0 = - \int d^3x \; \vec{\nabla} \cdot \vec{j} = - \oint \vec{n} \cdot \vec{j} \qquad (6.31)$$

The ~~cha~~ charge $\int d^3x \; \rho$ is a constant in time,

$$\rho = \frac{1}{c} j^0 = \frac{i\hbar}{2mc^2} \left(\varphi^* \partial_t \varphi - \varphi \partial_t \varphi^* \right) \qquad (6.32)$$

if the current vanishes at spatial infinity.

This seems to make ρ a perfect candidate for a probability density analogously to $\psi^* \psi$ in non relativistic QM.

However, there is a problem: as the Klein-Gordon equation is a 2nd-order differential equation, a solution requires ϕ and $\partial_t\phi$ as initial conditions at an initial time t_0. Since there are a priori no restrictions on ϕ and $\partial_t\phi$ at t_0, ρ in (6.32) can acquire any sign, positive or negative. Hence, ρ cannot be a probability density. Instead,

$e\rho$ is interpreted as an electric charge density (with e denoting a unit of charge) and the charge conservation then corresponds to the conservation of electric charge.

This has far reaching consequences: for a given charged particle with wave function ϕ and a positive charge density, we have to postulate the existence of a corresponding anti-particle with negative charge density (which allows and explains the occurrence of a negative charge density). In particular, if an initially positive charge density at t_0 evolves to a charge density with negative parts (say localized in some spacetime region), we can't interpret the solution ~~...~~ in terms of one-particle quantum mechanics, as an initial one-particle system has evolved into a system with anti-particle contributions.

In fact, relativistic one-particle QM does not exist (strictly speaking), but goes along with a transition to actually infinitely many degrees of freedom (as formalized within quantum field theory.)

Let us finally note that (6.32) actually is identically zero for real fields $\varphi \in \mathbb{R}$. This is consistent with the charge density interpretation (if we associate real fields with neutral particles, say π^0) but would be inconsistent with a probability density interpretation.

Positive / negative energy states

Another problem of the Klein-Gordon equation — if considered as analogous to the Schrödinger equation — is the occurrence of negative energy states.

For instance, a free particle in rest $p^\mu = (mc, \vec{0}) = (\hbar\mu, \vec{0})$ obeys

$$\partial_0^2 \varphi = \frac{1}{c^2} \partial_t^2 \varphi = -\mu^2 \varphi. \qquad (6.33)$$

Solutions are of the form $\sim e^{\pm i\mu ct}$. According to the correspondence rule $E \Rightarrow i\hbar\partial_t$, both signs of the energy appear. Solutions with positive energy are given by

$$\phi = e^{-i\mu ct} \,. \tag{6.34}$$

A transformation into a system moving at relative velocity $-\vec{v}$ implies for the wave function a change of 4-momentum

$$p^\mu \to p^{\mu\prime} = \left(\frac{E'}{c}, \vec{p}'\right) = \gamma m (c, \vec{v}) \,, \tag{6.35}$$

such that the new wave function is

$$\phi'(x') = \phi(x) = e^{-i\mu ct} = e^{-\frac{i}{\hbar}p_\mu x^\mu} = e^{-\frac{i}{\hbar}p'_\mu x^{\mu\prime}}$$
$$= e^{\frac{i}{\hbar}(\vec{p}'\cdot\vec{x}' - E't')} \,. \tag{6.36}$$

Dropping the primes, the corresponding 4-current is

$$\rho = \frac{E}{\mu c^2} \quad \text{and} \quad \vec{j} = \frac{\vec{p}}{m} = \rho\vec{v} \,, \tag{6.37}$$

with the plausible result that the current equals the density times velocity.

The other solution

$$\phi = e^{+imct} \tag{6.38}$$

describes a particle at rest with negative energy and density $\rho = -1$. The Lorentz-Boosted wave function is

$$\phi = e^{-\frac{i}{\hbar}(\vec{p}\cdot\vec{x} - |E|t)}$$

where
$$|E| = \sqrt{\vec{p}^2 c^2 + m^2 c^4} \tag{6.39}$$

The corresponding 4-current is

$$\rho = -\frac{|E|}{mc^2} \quad \text{and} \quad j = -\frac{\vec{P}}{m} = \rho\vec{v}. \tag{6.40}$$

Both problems, negative probabilities and negative energies, can be "solved" by reinterpreting these quantities in terms of anti-particles with positive energy and opposite charge. Formally, this reinterpretation can be realized by saying that the anti-particle has negative energy but evolves backward in time

$$e^{+ipct} = e^{-\frac{i}{\hbar}|E|(-t)} \tag{6.41}$$

Note that also g changes sign if t is reversed

$$g(-t) = -g(t) . \qquad (6.42)$$

Again, we stress that this consistent reinterpretation requires to leave the realm of one-particle QM but goes along with an a priori unbounded number of (anti-) particles.

6.3 Coupling to the electromagnetic field

In both mechanics and quantum mechanics, a Hamiltonian system can be put into an external electromagnetic field by replacing

$$E \Rightarrow E - e\phi \quad , \vec{p} \Rightarrow \vec{\pi} = \vec{p} - \frac{e}{c}\vec{A} \, , \qquad (6.43)$$

where ϕ is the electrostatic potential and $\vec{A}$ the vector potential. In order to avoid confusion with the wave function, let us rename the electrostatic potential $\phi \to A^0$, such that the potentials are summarizable in a 4-potential $A^\mu = (\phi, \vec{A})$.

Then (6.43) reads

$$p_\mu \Rightarrow p_\mu - \frac{e}{c} A_\mu \xrightarrow[\text{rule}]{\text{correspondence}} i\hbar \left(\partial_\mu + \frac{ie}{\hbar c} A_\mu\right) \qquad (6.44)$$

Here we encounter the covariant derivative

$$D_\mu := \partial_\mu + \frac{ie}{\hbar c} A_\mu \qquad (6.45)$$

which plays an important role in relativistic gauge theories. The attribute "covariant" arises from the transformation property under gauge transformations $A_\mu \to A'_\mu = A_\mu - \partial_\mu \lambda$ (6.46)

$$D_\mu(A') = \partial_\mu + \frac{ie}{\hbar c} A'_\mu = e^{\frac{ie}{\hbar c}\lambda} \left(\partial_\mu + \frac{ie}{\hbar c} A_\mu\right) e^{-\frac{ie}{\hbar c}\lambda}$$

$$= e^{\frac{ie}{\hbar c}\lambda} D_\mu(A)\, e^{-\frac{ie}{\hbar c}\lambda}, \qquad (6.47)$$

such that D_μ transforms under gauge rotations by phase rotations (similar to wave functions). Note that the commutator of two D's yields

$$[D_\mu, D_\nu] = \frac{ie}{\hbar c} (\partial_\mu A_\nu - \partial_\nu A_\mu) = \frac{ie}{\hbar c} F_{\mu\nu} \qquad (6.48)$$

with the electromagnetic field strength tensor

$$F_{\mu\nu} = \begin{pmatrix} 0 & E_1 & E_2 & E_3 \\ -E_1 & 0 & -B_3 & B_2 \\ -E_2 & B_3 & 0 & -B_1 \\ -E_3 & -B_2 & B_1 & 0 \end{pmatrix} \qquad (6.49)$$

on the right-hand side.

Inversely,

$$
\begin{aligned}
E_i &= F_{0i} \\
B_i &= -\frac{1}{2}\,\varepsilon_{ijk}\,F_{jk}
\end{aligned}
\qquad (6.50)
$$

The Klein-Gordon equation in an electromagnetic field is then obtained by simply replacing derivatives by covariant derivatives:

$$\left(D_\mu D^\mu + \mu^2\right)\phi = \left(g^{\mu\nu} D_\mu D_\nu + \frac{m^2c^2}{\hbar^2}\right)\phi = 0 \,. \qquad (6.51)$$

From the covariance property (6.47) of D_μ, we can infer that if $\phi(x)$ solves the Klein-Gordon equation for a gauge potential A_μ, then

$$\phi'(x) = e^{\frac{ie}{\hbar c}\lambda(x)}\,\phi(x) \qquad (6.52)$$

solves the Klein-Gordon equation with a gauge-transformed potential A'_μ. (NB: note that a coupling to the electromagnetic field requires $\phi \in \mathbb{C}$; otherwise, the gauge invariance cannot be maintained.)

This suggest a connection between complex conjugation and anti-matter: note that if ϕ satisfies (6.51), ϕ^* satisfies the same equation with e replaced by $-e$, as complex conjugation of the covariant derivative

$$D_\mu^* = \left(\partial_\mu + \frac{ie}{\hbar c} A_\mu\right)^* = \partial_\mu - \frac{ie}{\hbar c} A_\mu$$

$$= \partial_\mu + \frac{i(-e)}{\hbar c} A_\mu \qquad (6.53)$$

can be intepreted as charge conjugation $e \Rightarrow -e$.

Generally, we can define the <u>charge conjugation</u> as a transformation of the fields:

$$\phi(x) \Rightarrow \phi_c(x) = \phi^*(x). \qquad (6.54)$$

6.3 Pionic atoms

With these reservations concerning probability and energy interpretations in mind, we can use the Klein-Gordon equation for determining the spectrum of a scalar particle, say a negatively charged pion π^-, in the Coulomb field of an (infinitely) heave nucleus.

As the potential is considered to be static, we make a stationary ansatz,

$$\Phi(t,\vec{x}) = e^{-i\frac{E}{\hbar}t}\,\varphi(\vec{x}) \tag{6.55}$$

for the positive energy solutions (we do not expect bound states for positively charged antimatter, π^+, in a Coulomb field of a positively charged nucleus).

The charge density then yields

$$e\rho = \frac{e}{mc^2}\left(E - eA_0(\vec{x})\right)|\varphi(\vec{x})|^2. \tag{6.56}$$

For a π^-, e is defined as negative here. Also $A_0 < 0$. Hence the charge density $e\rho$ has the same sign as e in the classically allowed region

$$E > eA_0(\vec{x}) \tag{6.57}$$

and the opposite sign in the classically forbidden region

$$E < eA_0(\vec{x}). \tag{6.58}$$

Hence, the wave function is a superposition of matter and anti-matter states with matter dominating in the classically allowed region, and anti-matter "being attracted" towards the classically forbidden region.

Actually for antimatter $e \to -e$ such that what is classically allowed for matter, is forbidden for antimatter and vice versa.

Again, what we find here and have just described is a "classical" many body effect: "polarization". However, as we are dealing with a one-particle problem in a Coulomb field which is otherwise in vacuum, this phenomenon is also dubbed "vacuum polarization".

For the pionic atom, we have

$$e A_0 = -\frac{Ze^2}{r} \quad \text{and} \quad A_i = 0 \quad , \; r = |\vec{x}|. \tag{6.59}$$

The Klein-Gordon equation then reads

$$\left(D_0^2 - \vec{\nabla}^2 + \mu^2\right) \phi(t,\vec{x}) = 0 . \tag{6.60}$$

Using the stationary ansatz (6.55), we find

$$\left(E + \frac{Ze^2}{r}\right)^2 \phi(\vec{x}) + \hbar^2 c^2 \vec{\nabla}^2 \phi(\vec{x}) - m^2 c^4 \phi(\vec{x}) = 0 . \tag{6.61}$$

Due to spherical symmetry, we decompose as usual

$$\Phi(\vec{x}) = f_{n\ell}(r)\, Y_{\ell m}(\theta, \varphi) \qquad (6.62)$$

Using $r^2 \vec{\nabla}^2 = r\,\partial_r^2\, r - \vec{L}^2$, the radial Klein-Gordon equation for the radial wave function $f_{n\ell}(r)$ reads

$$\left(\frac{E^2}{c^2} - m^2 c^2\right) f_{n\ell} + \hbar^2 \left(\frac{1}{r}\partial_r^2 r - \frac{\ell(\ell+1) - (Z\alpha)^2}{r^2}\right) f_{n\ell}$$

$$+ \frac{2Ze^2}{r}\,\frac{E}{c^2}\, f_{n\ell} = 0 \qquad (6.63)$$

where $\alpha = \dfrac{e^2}{\hbar c}$ is the fine structure constant in our present units.

In order to bring this differential equation into a known form, we shift

$$\begin{aligned}
&\text{angular momentum} && \ell'(\ell'+1) := \ell(\ell+1) - (Z\alpha)^2 \\
&\text{mass} && m' := \frac{E}{c^2} \qquad\qquad (6.64)\\
&\text{energy} && 2m'E' := \frac{E}{c^2} - m^2 c^2 ,
\end{aligned}$$

yielding

$$\left(2m'E' + \frac{\hbar^2}{r}\partial_r^2 r - \hbar^2 \frac{\ell'(\ell'+1)}{r^2} + \frac{2m'Ze^2}{r}\right) f_{n\ell} = 0 \qquad (6.65)$$

This looks identical to the radial Schrödinger Coulomb problem with the important difference that l' is not an integer. The generalization of the Schrödinger-type solution (~ Laguerre polynomials times exponentials) are the so-called Whittaker fuctions.

Solving the resulting eigenvalues E' for E, results in

$$E = \frac{mc^2}{\sqrt{1+\left(\frac{Z\alpha}{n'}\right)^2}} \tag{6.66}$$

where

$$n' = l' + 1 + \underset{\substack{\uparrow \\ \text{radial} \\ \text{quantum} \\ \text{number}}}{\nu}, \quad \nu = 0, 1, 2, \ldots$$

and $$l' = -\frac{1}{2} + \sqrt{(l+\tfrac{1}{2})^2 - (Z\alpha)^2}, \quad l = 0, 1, 2, \ldots \tag{6.67}$$

So, l' and E are only real, as long as

$$(l+\tfrac{1}{2})^2 > (Z\alpha)^2 \iff Z < \frac{1}{2\alpha} \sim \frac{137}{2} \tag{6.68}$$

In order to illustrate the relation the the standard hydrogen spectrum, we introduce the principal quantum number $n = l+1+\nu$ of the latter, and find

$$n' = (\nu + l + 1) - (l+\tfrac{1}{2}) + \sqrt{(l+\tfrac{1}{2})^2 - (Z\alpha)^2}$$

$$= n - (l+\tfrac{1}{2}) + \sqrt{\cdots} \quad , \; n = l+1, l+2, l+3, \ldots \tag{6.69}$$

For small $Z\alpha$, we may expand in powers of the fine-structure constant and find

$$E_{nl} \simeq mc^2 - \underbrace{\frac{Z^2 e^2}{2an^2}}_{} \left(1 + \frac{Z^2\alpha^2}{n^2}\left(\frac{n}{l+\frac{1}{2}} - \frac{3}{4}\right)\right) \tag{6.70}$$

Bohr radius (for a pion)

We discover the rest mass energy $\sim mc^2$, the standard hydrogen-like spectrum $\sim \frac{Z^2 e^2}{2an^2}$, and a relativistic correction. The latter lifts the degeneracy with l and thus determines the fine-structure. Apart from quantum-field theoretic corrections (vacuum polarization) and corrections due to the strong interactions of nuclei with pions (which are short range), this formula describes the experimentally determined spectrum very well.

(E.g.: binding energy of the 1s state: 3235.156 eV

corrections from vacuum polarization to order α^2: 3,246 eV

corrections from p and π^- form factors (p and π^- are not point particles): $-$0.102 eV)