– From Einstein to Klein-Gordon – Quantum Mechanics and Relativity

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March 24, 2002

Abstract

We study the development from Einstein's relativistic energy-momentum relation for free particles, $E^2 - c^2\vec{p}^{\,2} - m_0^2c^4 = 0$, to the Klein-Gordon equation, $[-\hbar^2\partial_t^2 + c^2\hbar^2\Delta - m_0^2c^4]\psi = 0$, describing free spin-less particles in quantum mechanics (QM). To this end, we will introduce concepts of QM motivated by de Broglie's particle-wave dualism ("$\vec{p} = \hbar\vec{k}$") and Einstein's explanations of the photo electric effect ("$E = \hbar\omega$"). We show explicitly the Lorentz invariance of the Klein-Gordon equation and contrast this with the non-relativistic free Schrödinger equation $[i\hbar\partial_t + \hbar^2/(2m)\Delta]\psi = 0$.

1 Introduction into Quantum Mechanical Phenomena

In this section we discuss fundamental physical observations which led to the development of a new theory, the *quantum mechanics*. We introduce Einstein's quantum hypothesis to describe the photoelectric effect and de Broglie's ansatz to understand particles as wave objects. These form the basis of (relativistic) quantum mechanics and are of untold importance.

In 1905, Albert Einstein realized, motivated by the photoelectric effect, that the so called *quanta*, first used by Max Planck to describe that radiation were emitted in packets only, were not a feature of atoms but of light itself. Einstein therefore used *Planck's Law* for light and explained that one should think of the light as a stream of quanta (i.e., particles), the so called *photons*, whose energy E was proportional to their frequency ω,

$$E = \hbar\omega, \quad \hbar = 1.0546 \times 10^{-34}\,\text{Joule} \times \text{sec (Planck's constant)}. \tag{1}$$

The same year, Einstein developed his *special relativistic theory.* Within this theory he could relate the energy E of a free moving particle with its momentum $\vec{p}$ by claiming

$$\frac{E^2}{c^2} - \vec{p}^{\,2} = m_0^2 c^2, \tag{2}$$

where c is the speed of light and m_0 the rest mass of the particle. With Einstein's hypothesis about the particle character of light we can derive an energy-momentum relation for photons

$$E = c|\vec{p}|, \tag{3}$$

where we used that the photons' mass must be zero since they are propagating with speed of light.

At the other hand, some physical phenomena as the diffraction of light at small objects can only be explained by its wave character. We consider such a (non-interacting) planar light wave travelling in the direction $\vec{k}$ with a frequency ω,

$$\psi(\vec{x}, t) = e^{i\left(\vec{k}\cdot\vec{x} - \omega t\right)}. \tag{4}$$

The wave vector $\vec{k}$ and ω are related to the propagation speed c by $\omega = c|\vec{k}|$, i.e., the length $|\vec{k}|$ of the wave vector equals $2\pi/\lambda$ with λ being the wavelength of the light. From (1) and (3) follows that the momentum of a photon is proportional to its wave vector:

$$|\vec{p}| = \frac{\hbar\omega}{c} = \frac{\hbar\omega}{\omega/|\vec{k}|} = \hbar|\vec{k}|.$$

Since the momentum of the light is collinear with the propagation direction we even get

$$\vec{p} = \hbar\vec{k}. \tag{5}$$

Plugging this and (1) into (4) we get

$$\psi(\vec{x},t) \equiv \psi_{\vec{p}}(\vec{x},t) = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}(\vec{p}\cdot\vec{x}-Et)}, \tag{6}$$

where we additionally introduce a normalization factor whose convenience becomes clear in the next section.

The above considerations show that there exist two different, equally justified, models describing the structure of light. The connection between both models is given by (5).

In 1923-24, de Broglie did an experiment in which he sent electrons to a double slit. Surprisingly, he observed patterns on a screen behind which did not look like the projection of the slits via geometrical optics but rather like the interference structure of light waves diffracted at the same slit apparatus. Motivated by this, he claimed that electrons also behaved like waves and assigned to any particle with momentum $\vec{p}$ a wave vector $\vec{k}$ via (5).[1] Therewith he extended the particle-wave dualism of light to every kind of matter. Based on this we understand a free moving particle of momentum $\vec{p}$ and energy E as a planar wave of the form (6).

2 Mathematical Objects and Physical Interpretations in Quantum Mechanics

In this section we introduce the mathematical objects of quantum mechanics (henceforth abbreviated as QM) and give a physical meaning to them, e.g., we motivate how the assigned wave function (as figured out in the last section) of a particle describes its configuration. Further, we work out the dynamics of QM systems.

First, we recall the objects of Newton mechanics (NM) to contrast them later with QM. The configuration of a single particle in the three dimensional space is given by the pair $(\vec{x},\vec{p}) \in \mathsf{R}^3_{\vec{x}} \times \mathsf{R}^3_{\vec{p}}$ of position $\vec{x}$ and momentum $\vec{p}$. The Hilbert space $\mathcal{H} = \mathsf{R}^3_{\vec{x}} \times \mathsf{R}^3_{\vec{p}}$ of all possible configurations is the configuration space. The motion of such a particle with mass m obeys by

[1] The corresponding wavelength $\lambda = 2\pi\hbar/|\vec{p}|$ is known as *de Broglie wavelength* of the particle.

Newton's law a differential equation of the form

$$m\ddot{\vec{x}}(t) = F(\vec{x}(t), \dot{\vec{x}}(t)), \tag{7}$$

where $F(\vec{x}, \vec{v})$ is the force onto the particle at position $\vec{x}$ and velocity $\vec{v} = \vec{p}/m$. Since (7) is a differential equation of second order in t, two initial conditions on $\vec{x}(t)$ are needed in order to solve it uniquely, e.g., $\vec{x}(t_0) = \vec{x}_0$, $\dot{\vec{x}}(t_0) = \vec{p}_0/m$. Thus, the motion of the particle is determined by assigning a configuration $(\vec{x}_0, \vec{p}_0)$ to a given time t_0.

Physical observables are real valued functions

$$f : \mathcal{H} \to \mathsf{R} \tag{8}$$

assigning to a given position and momentum a measurable quantity of the system. An important example is the total energy observable

$$H(\vec{x}, \vec{p}) = \frac{\vec{p}^{\,2}}{2m} + V(\vec{x}), \tag{9}$$

where $\vec{p}^{\,2}/2m$ describes the (non-relativistic) kinetic energy and $V(\vec{x})$ the potential energy induced by the force F.

We now go over to describe configurations of QM systems. Thereby, we restrict ourselves to the spin-less description of particles. During the last section we have seen that a particle with momentum $\vec{p}$ can be associated with a planar wave $\psi_{\vec{p}}$ given in (6). We want to generalize this association. We consider configurations for a fixed time such that we drop – for the moment – the time dependence in (6) by setting $t = 0$. Assume we are given a momentum distribution $\hat{\psi} \in \mathcal{H}_{\vec{p}} := L^2(\mathsf{R}^3_{\vec{p}}; \mathsf{C})$, e.g., $\vec{p} \mapsto |\hat{\psi}(\vec{p})|^2/\|\hat{\psi}\|^2_{\mathcal{H}_{\vec{p}}}$ is the probability density that the particle possesses the momentum $\vec{p}$ ($\| \cdot \|_{\mathcal{H}_{\vec{p}}}$ denotes the L^2-norm of the Hilbert space $\mathcal{H}_{\vec{p}}$). To such a momentum configuration we assign a wave function $\psi \in \mathcal{H}_{\vec{x}} := L^2(\mathsf{R}^3_{\vec{x}}; \mathsf{C})$ by

$$\psi(\vec{x}) \equiv \psi_{\hat{\psi}}(\vec{x}) := \frac{1}{(2\pi\hbar)^{3/2}} \int\limits_{\mathsf{R}^3} \hat{\psi}(\vec{p}) e^{\frac{i}{\hbar}\vec{p}\cdot\vec{x}}\, d^3p$$

which is the superposition of planar waves $\psi_{\vec{p}}(\vec{x}, t = 0)$ weighted by $\hat{\psi}(\vec{p})$. Note that we recover (6) by choosing the delta-"function" as momentum distribution, $\hat{\psi}(\vec{p}\,') = \delta(\vec{p} - \vec{p}\,')$. We stress that the momentum distribution $\hat{\psi}$

and the wave function ψ are one-to-one related via the Fourier transformation $\mathcal{F} : \mathcal{H}_{\vec{x}} \to \mathcal{H}_{\vec{p}}$, given by

$$[\mathcal{F}\psi](\vec{p}) \equiv \hat{\psi}(\vec{p}) := \frac{1}{(2\pi\hbar)^{3/2}} \int\limits_{\mathbf{R}^3} \psi(\vec{x}) e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{x}}\, d^3x.$$

Therefore the wave functions ψ span the whole Hilbert space $\mathcal{H}_{\vec{x}}$. It remains to give physical significance to them. A non-zero element $\psi \in \mathcal{H}_{\vec{x}}$ describes the configuration of a single particle in the sense that $\vec{x} \mapsto |\psi(\vec{x})|^2/\|\psi\|^2_{\mathcal{H}_{\vec{x}}}$ is the probability density to find the particle at the position $\vec{x}$. It is crucial that ψ already carries information about the momentum distribution $\hat{\psi}$ since both are related by $\mathcal{F}$. This shows that all physical configurations are already encoded in $\mathcal{H}_{\vec{x}}$ or $\mathcal{H}_{\vec{p}}$, resp., and not by its product as in NM. Henceforth we will denote the configuration space by $\mathcal{H} := L^2(\mathbf{R}^3; \mathbf{C})$ and understand it as the space of configurations in either position or momentum representation, $\psi(\vec{x})$ or $\hat{\psi}(\vec{p})$, resp.

It seems convenient to define the mean position of a particle in a state $\psi(\vec{x})$ in position representation. The expectation value of the jth coordinate x_j in the state ψ is defined as

$$\langle X_j \rangle_\psi := \int\limits_{\mathbf{R}^3} x_j |\psi(\vec{x})|^2\, d^3x. \tag{10}$$

Using that the inner product on the Hilbert space $\mathcal{H}$ is given by $\langle \varphi, \phi \rangle = \int_{\mathbf{R}^3} \overline{\varphi(\vec{x})} \phi(\vec{x})\, d^3x$ we can write (10) as

$$\langle X_j \rangle_\psi = \langle \psi, X_j \psi \rangle\,,$$

where X_j is the *position operator* on $\mathcal{H}$ defined by

$$[X_j \psi]\,(\vec{x}) := x_j \psi(\vec{x}).$$

Similarly, we get the expectation value of the jth coordinate of the momentum, p_j, in the state ψ by

$$\langle P_j \rangle_\psi := \int\limits_{\mathbf{R}^3} p_j |\hat{\psi}(\vec{p})|^2\, d^3p,$$

where $\hat{\psi} = \mathcal{F}\psi$ is the momentum representation. We can express this in terms of a *momentum operator* P_j,

$$\langle P_j \rangle_\psi = \langle \psi, P_j \psi \rangle \,,$$

where P_j must fulfil $\mathcal{F}\left[P_j\psi\right](\vec{p}) := p_j\hat{\psi}(\vec{p})$. It is easy to see that

$$\left[P_j\psi\right](\vec{x}) = -i\hbar\partial_{x_j}\psi(\vec{x}).$$

In what follows, we abbreviate the three components of position and momentum operator by $\vec{X}$ and $\vec{P}$, resp.

The physical observables in a QM framework are described as operators on $\mathcal{H}$ which are built of position and momentum operators. The procedure which assigns an operator $f(\vec{X}, \vec{P})$ to a classical observable given in (8) is called *quantization*. The most important example for our purposes is the quantization of the total energy observable (9),

$$H \equiv H(\vec{X}, \vec{P}) = \frac{\vec{P}^{\,2}}{2m} + V(\vec{X}) = -\frac{\hbar^2}{2m}\Delta + V(\vec{X}),$$

where $\vec{P}^{\,2} := P_1^2 + P_2^2 + P_3^2$ and $V(\vec{X})$ is an operator only dependent upon the position operator. We get the kinetic energy operator by setting $V(\vec{X}) = 0$.

We want to describe the dynamics for a QM system. To this end we have to find a differential equation which is solved for a family of configurations $\psi(\,\cdot\,,t) \in \mathcal{H}$ labelled by the time parameter t describing the actual motion of the system. Since the configuration of the system for an initial time $t = t_0$ is totally determined by a wave function ψ_0 the evolution $t \mapsto \psi(\,\cdot\,,t)$ must uniquely be given by the wanted differential equation and the initial condition $\psi(\,\cdot\,,t_0) = \psi_0$. This implies that the equation of motion must be of first order in derivatives w.r.t. the time variable t, i.e., of the form

$$i\hbar\partial_t\psi(\,\cdot\,,t) = F\left(\psi(\,\cdot\,,t)\right), \tag{11}$$

where F is a function on $\mathcal{H}$. To fix the map F we recall that the description of interference phenomena for (material) wave functions must be contained in the dynamics , i.e., we require the superposition principle for the equation (11). In other words, we require that (11) is a linear equation. This makes necessary that $F(\psi) = H\psi$ is a linear operator, the so called *Hamilton operator*, on $\mathcal{H}$. The equation (11) now reads

$$i\hbar\partial_t\psi(\,\cdot\,,t) = H\psi(\,\cdot\,,t) \tag{12}$$

and is known as *Schrödinger equation*.

To stress the physical significance of the Hamilton operator H we plug the (planar) wave function $\psi_{\vec{p}}(\vec{x}, t)$ given in (6) for a free particle into the Schrödinger equation (12) and get

$$E\psi_{\vec{p}}(\,\cdot\,, t) = H\psi_{\vec{p}}(\,\cdot\,, t) \tag{13}$$

which is an eigenvalue equation for H. Since E is the energy of the free (planar) wave it is suggestive that H is the kinetic energy operator $H = \vec{P}^{\,2}/(2m) = -\hbar^2/(2m)\Delta$. This together with (13) leads to the energy-momentum relation

$$E = \frac{\vec{p}^{\,2}}{2m} \tag{14}$$

as one expects for free (non-relativistic) particles. With these considerations the free Schrödinger equation has the form

$$i\partial_t\psi(\vec{x}, t) = -\frac{\hbar^2}{2m}\Delta\psi(\vec{x}, t) \tag{15}$$

and its solutions are the planar waves (6) fulfilling (14). To describe the dynamics of particles in a potential $V(\vec{x})$ we have to modify the free Hamilton operator to $H = \vec{P}^{\,2}/(2m) + V(\vec{X})$ and result in the interacting Schrödinger equation

$$i\partial_t\psi(\vec{x}, t) = \left[-\frac{\hbar^2}{2m}\Delta + V(\vec{x})\right]\psi(\vec{x}, t). \tag{16}$$

3 Non-Invariance of the Free Schrödinger Equation under Lorentz Transformation

In this section we will show that the Schrödinger equation is not a relativistic one. This results in the fact that the energy-momentum relation (14) of solutions of the free Schrödinger equation (planar waves) is not a relativistic relation. To understand where the relativistic character of the Schrödinger equation fails we show that it is not form invariant under Lorentz transformations. This is done at a concrete example.

Let

$$\mathcal{L} := \left\{\Lambda \in \mathsf{R}^{4\times 4}\;\middle|\Lambda^T g\Lambda = g\right\} \tag{17}$$

be the group of Lorentz transformation, where the Minkowski metric g is given by

$$g = \begin{pmatrix} -1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

We denote for a given Lorentz transformation Λ

$$x' := \Lambda x, \tag{18}$$

where $x = (x_0 = ct, \vec{x})$ is the four-position vector. The transformation Λ can be lifted to the wave functions $\psi(\vec{x}, t) \equiv \psi(x)$ by

$$\psi'(x') := \psi(x) = \psi(\Lambda^{-1} x'). \tag{19}$$

The transformation of the four-gradient $\nabla = (\partial_0, \ldots, \partial_3)$ obeys

$$\partial_\mu \psi(x) = \sum_{\nu=0}^{3} \partial'_\nu \psi'(x') \frac{\partial x'_\nu}{\partial x_\mu} = \sum_{\nu=0}^{3} \partial'_\nu \psi'(x') \Lambda_{\nu\mu} = \left[\Lambda^T \nabla'\right]_\mu \psi'(x') \tag{20}$$

and consequently

$$\partial_\mu \partial_\tau \psi(x) = \sum_{\nu,\sigma=0}^{3} \Lambda_{\nu,\mu} \Lambda_{\sigma,\tau} \partial'_\nu \partial'_\sigma \psi'(x'). \tag{21}$$

Lorentz invariance of the free Schrödinger equation

$$\left[ic\hbar\partial_0 + \frac{\hbar^2}{2m}(\partial_1^2 + \partial_2^2 + \partial_3^2)\right] \psi(x) = 0 \tag{22}$$

would mean that we can replace the variable x, the wave function ψ and the partial derivatives ∂_μ by their transformed analogues x', ψ' and ∂'_μ and get an equation still describing the same dynamical system. Since the temporal and the spatial derivatives in (22) do not appear in the same order we see directly that temporal and spatial coordinates are not treated equally within the theory. To show in details that Lorentz invariance fails in the case of the Schrödinger equation we specify our choice of a Lorentz transformation to be a pure Lorentz boost,

$$\Lambda := \begin{pmatrix} \cosh\theta & \sinh\theta & 0 & 0 \\ \sinh\theta & \cosh\theta & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix},$$

with $\theta \neq 0$, which mixes time and spatial coordinates.[2] It follows immediately that

$$\begin{aligned}
\partial_0 &= \cosh(\theta)\partial_0' + \sinh(\theta)\partial_1', \\
\partial_1 &= \sinh(\theta)\partial_0' + \cosh(\theta)\partial_1', \\
\partial_2 &= \partial_2' \\
\partial_3 &= \partial_3'.
\end{aligned}$$

Therefore, the Schrödinger equation (22) transforms under Λ to

$$\Big[\frac{\hbar^2}{2m}\left(\sinh^2(\theta)\partial_0'^2 + \cosh^2(\theta)\partial_1'^2 + 2\sinh(\theta)\cosh(\theta)\partial_0'\partial_1' + \partial_2'^2 + \partial_3'^2\right) \\ + ic\hbar\left(\cosh(\theta)\partial_0' + \sinh(\theta)\partial_1'\right)\Big]\psi'(x') = 0$$

which is not of the form (22). This shows that the free Schrödinger equation is not Lorentz invariant and does not qualify for the description of relativistic quantum mechanics. In the next section we will modify the Schrödinger equation to get an Lorentz invariant expression.

4 The Klein-Gordon Equation

The requirement on a relativistic description of QM is an equation for wave functions $\psi(x)$ which is form invariant under Lorentz transformations $\Lambda \in \mathcal{L}$ (defined in (17)) in the sense mentioned in the last section. We have seen that this in particular demands that the time and spatial variables are treated in the same way and therefore temporal and spatial derivatives of the wanted wave equation must appear in the same order. In this section we develop an equation for non-interacting waves which gives the right relativistic energy-momentum relation of free particles. Further, we prove that this equation is indeed Lorentz invariant.

In section 2 we have seen that we can obtain the free Schrödinger equation (15) by quantizing the non-relativistic energy-momentum relation (14). To this end we had to replace $\vec{p}$ formally by the 3-momentum operator $\vec{P}$ and

[2] One can check that pure rotations which only transform spatial coordinates among each other leave (22) form invariant.

E/c by the operator $i\hbar\partial_0 =: P_0$ which we will refer to from now on as the zero component of the 4-momentum operator $P = (P_0, \vec{P})$.

The canonical ansatz to find a Lorentz invariant wave equation is to quantize the relativistic energy-momentum relation (2) for free particles,

$$\left[-\hbar^2\partial_0^2 + \hbar^2\Delta + m_0^2c^2\right]\psi(x) = 0. \tag{23}$$

We introduce the notation of the *d'Alembert operator*, $\Box := \nabla^T g \nabla = \Delta - \partial_0^2$ (where $\nabla = (\partial_0, \ldots, \partial_3)^T$ is the 4-gradient written as a column) to write (23) in a compact form,

$$\left[\Box + \left(\frac{m_0 c}{\hbar}\right)^2\right]\psi(x) = 0. \tag{24}$$

This equation is the free *Klein-Gordon equation* which describes the (free) quantum dynamics of relativistic (spin-less) particles. It is suggestive that (24) is invariant under Lorentz transformations Λ because the operator $\Box$ is formally a Lorentz scalar. We will stress this in detail.

Let $\Lambda \in \mathcal{L}$ be a Lorentz transformation and recall from (18) – (21) the transformation of x, ψ and ∂_μ induced by Λ. We then have

$$\begin{aligned}
\Box\psi(x) &= \sum_{\mu,\tau=0}^{3} \partial_\mu g_{\mu,\tau} \partial_\tau \psi(x) \\
&= \sum_{\mu,\tau,\nu,\sigma=0}^{3} \Lambda_{\nu,\mu} g_{\mu,\tau} (\Lambda^T)_{\tau,\sigma} \partial'_\nu \partial'_\sigma \psi'(x') \\
&= \sum_{\nu,\sigma=0}^{3} (\Lambda g \Lambda^T)_{\nu,\sigma} \partial'_\nu \partial'_\sigma \psi'(x') \\
&= \sum_{\nu,\sigma=0}^{3} g_{\nu,\sigma} \partial'_\nu \partial'_\sigma \psi'(x') \\
&= \Box'\psi'(x'),
\end{aligned}$$

where we used that $\Lambda^T g \Lambda = g$ implies

$$\Lambda g \Lambda^T = \Lambda g (g \Lambda^{-1} g^{-1}) = g.$$

Together with (19) we end up with

$$\left[\Box' + \left(\frac{m_0 c}{\hbar}\right)^2\right]\psi'(x') = 0.$$

After having shown that the Klein-Gordon equation carries the features of a relativistic equation we are now interested in its solutions. As for the Schrödinger equation the planar waves

$$\psi_p(x) = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar} p \cdot x} \tag{25}$$

with a sharp 4-momentum $p = (E/c, \vec{p})$ (we use the notation $p \cdot x := \vec{p} \cdot \vec{x} - p_0 x_0$) are the solutions for the Klein-Gordon equation. However, as one can check by plugging (25) into (24), we get as energy momentum relation

$$p \cdot p + m_0^2 c^2 = 0$$

which is exactly the equation (2). We mention that – in contrast to the non-relativistic case (14) – the energy of solutions of the Klein-Gordon equation can also be negative,

$$E_\pm = \pm c \sqrt{\vec{p}^2 + m_0^2 c^2}.$$

The solutions yielding negative energy E_- are physically connected with antiparticles. It is impressionable that the relativistic description of quantum mechanics already predicts the existence of antiparticles.

We close this section with a remark. Choosing $m_0 = 0$ in (24) one get the wave equation as it appears in electro dynamics. This is consistent with the fact that the relativistic quantum mechanical description of (massless) photons should be the same as described by *Maxwell's equations.*

5 Lacks of the Klein-Gordon Equation and Outlook

In this section we will state some lacks of the Klein-Gordon equation. From (23) it is obvious that the Klein-Gordon equation is of second order w.r.t. the time derivative. This implies that the dynamics of the system described by (24) is not determined by a single initial condition $\psi(\,\cdot\,, t_0) = \psi_0$ but rather we have to require an additional condition on $\partial_t \psi(\,\cdot\,, t_0) = \dot{\psi}_0$. Consequently, a single wave function $\psi_0 \in \mathcal{H}$ cannot encode the whole information of the system's configuration since it does not allows predictions of the configuration at later times $t > t_0$. To remove this weakness one can write the Klein-Gordon equation as two coupled Schrödinger equations where we also split the wave function $\psi = (\varphi, \chi)$ into two components referring to its part with positive energy (particle), φ, and negative energy (antiparticle), χ.[3]

Further, the Klein-Gordon equation is not qualified for describing spin-1/2 particles. The relativistic description of spin particles requires a totally new investigation which leads to the *Dirac equation*.[4]

Acknowledgment: The author wants to thank Matthias for fruitful discussions and his supporting help.

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[3] for details see [Gr]

[4] see [Ha]