

Klein-Gordon field equation

existence and uniqueness of solutions

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Abstract

We aim to prove existence and uniqueness of solutions to the initial value problem of the Klein-Gordon (K-G) equation $(\square + m^2)\psi = 0$. For this we properly introduce the mathematical framework and motivation for deriving the K-G equation, including the basics of quantum mechanics and special relativity. We derive the energy to show uniqueness and use Fourier transformations for existence.

Historical background

Since their discovery around the beginning of the 20th century, special relativity and quantum mechanics have been astonishingly insightful, useful and complicated topics in physics and mathematics. While being quite non-intuitive and dense, they have beautiful properties and interesting experimental results.

To lay the background for the motivation of each we start from Newtonian relativity¹ and Newtonian mechanics, both built upon axioms of absolute space and time and simultaneity of events [Cho15, §2.2]. These theories worked quite flawlessly² for around 200 years, with their working principles based upon the group of Galilean transformations.

However, around the nineteenth-century, Maxwell developed and unified the laws for electromagnetic fields (Maxwell equations (*see Appendix 1*)). In other words, he discovered a way of describing the electric field and the magnetic field, and how they evolve and relate to each other. The problem arises from considering the behavior of charged particles, as their motion should have followed or translated into Newtonian mechanics, and that meant being invariant under the Galilean group of transformations, but Maxwell equations were not. A few years later a new group (the Lorentz group (*see 8*)) was formulated, upon which these equations are invariant. However this transformation clashes with the notion of simultaneity, as there is a co-dependence of space and time. This is where special relativity comes in to 'shake' our understanding of the universe (*see 2.3*).

Now, the motivation for quantum mechanics arises as a result of the photoelectric effect and the double slit experiment, which showed that light is quantized (it comes in packets called photons) and that it behaves both as a wave and as a particle depending on the observer effect³. It also showed that the excitement of atoms is quantized in the same manner, so in the notion we had about atom structures at the time, electrons jumped states in a countable fashion, i.e. energy is quantized. This two facts started a massive branch of physics, the physics of quantifiable objects or quantum physics.

¹Or Galilean, used interchangeably.

²Up to an approximation that was pretty much unmeasurable at the time.

³The fact that its probability of being somewhere or not 'collapses' upon being measured. More in section 2.2.

If we want to talk about motion and positions in this context we encounter a fundamental issue when relating it to Newtonian mechanics, which is that quantum mechanics does not follow Boolean algebra [Fol08, §3.1 p.]. In a quantum system there is no notion of true and false states per se, but rather a probability distribution between them. In other words you cannot know the state a system is in, but rather the probability of it being in one or the other. A second extremely common and useful notion is obtained from the quantum harmonic oscillator and how it relates to the classical case [Fol08, §3.4]. Due to the uncertainty principle ($\Delta x \Delta p \geq \frac{\hbar}{2}$) obtained from the standard deviation of two non-commuting self-adjoint operators [Fol08, §3.3] we have that the solution to the standard harmonic oscillator does not really make sense inside the quantum realm, as we cannot specify both position and momentum at the same time with accuracy, something we are 'able' to do in a classical sense (to an approximation as the uncertainty principle remains true, yet, as classically we work in SI units, the error is very small).

1 Introduction

The Klein–Gordon equation is often introduced as a relativistic generalization of the Schrödinger equation. While this perspective is historically motivated, it does not capture the full mathematical structure under its formulation nor the tools required to understand its behavior. We aim to approach the Klein–Gordon equation not only from a physical point of view, but as a consequence of treating certain differential operators as self-adjoint operators on a Hilbert space.

The central sections of this work focus on the mathematical formulation of the Klein–Gordon equation. We explore the functional-analytic framework that allows us to derive existence and uniqueness of solutions, particularly by using Fourier transforms and energy estimates. The use and necessity for unbounded self-adjoint operators and Hilbert space methods becomes apparent.

The aim is to provide a minimal yet coherent path from the physical motivations of the Klein–Gordon equation to a more rigorous mathematical formulation. The first part of the essay serves as a background introduction while the later sections establish the main analytical results.

2 Background

It is in order now for us to introduce some of the background that sets up the Klein-Gordon equation. Refer to [Fol08] for further information.

We will also briefly introduce special relativity and quantum mechanics. The historical background gave some motivation for each, now it is time for the mathematical side.

2.1 Mathematical background

We start introducing the required knowledge for a mathematical foundation of quantum mechanics:

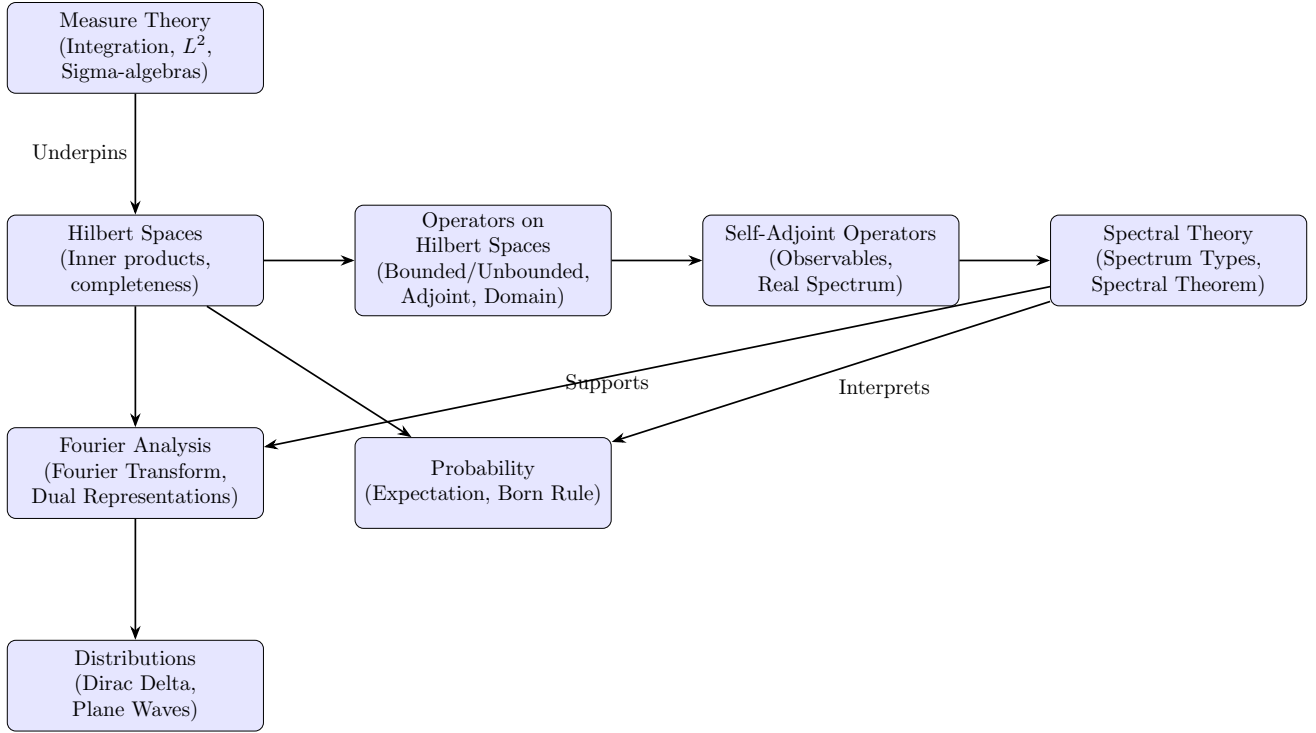


Figure 1: Diagram showcasing the relation between different mathematical concepts used in QM.

2.1.1 For Quantum Mechanics

The mathematical structure of quantum mechanics is based on unbounded self adjoint operators on Hilbert spaces. Figure 1 shows some insight into how different topics relate and connect. We will introduce some definitions with our base on this textbook [Sch12].

Definition 1. (Hilbert L^2 space)

Let $\Omega \subseteq \mathbb{C}^n$. We define a complex Hilbert space $\mathcal{H} = L^2(\Omega)$ as a Banach space (See 5.2) endowed with an inner product $\langle \cdot, \cdot \rangle$ defined as:

$$\langle u, v \rangle = \int_{\Omega} u \cdot \bar{v} \, dx, \quad u, v \in \mathcal{H}(\Omega) \quad (1)$$

Which is linear in the first variable and conjugate-linear in the second [Bla06, §I.1.1]. This generates the norm $\|v\|_{\mathcal{H}(\Omega)}^2 = \langle v, v \rangle$.

Definition 2. (Linear Operators)

Let $\mathcal{H}_1, \mathcal{H}_2 \subset \mathcal{H}$ be Hilbert spaces on Ω . Linear (differential) operators are linear mappings from \mathcal{H}_1 to \mathcal{H}_2 . Let A be an operator, then $\mathcal{H}_1 := D(A)$ is the domain of A and $\mathcal{H}_2 := R(A)$ is its range. In QM we will deal with maps from \mathcal{H} onto itself, i.e. $D(A) = R(A)$.

Definition 3. (Self-Adjoint Operators)

Let A be an operator, we define A^* the adjoint operator of A , with the property that:

$$\langle Au, v \rangle = \langle u, A^* v \rangle, \quad u, v \in \mathcal{H}(\Omega). \quad (2)$$

If it holds that $A = A^*$, then the operator is *Self-Adjoint*. Furthermore if $A = A^* = A^2$, then the operator is called a *projection*.

Theorem 1. (Spectral Theorem)

Let A denote a self-adjoint operator, then there exists a unique spectral measure $E = E_A$ on the Borel σ -algebra (See Appendix (5.2)) $\mathcal{B}(\mathbb{C})$, such that:

$$A = \int_{\Omega} \lambda dE_A(\lambda) \quad (3)$$

In simpler terms, if A is a self-adjoint operator, the spectral theorem states that it can be diagonalized, i.e. written as the integral sum of orthogonal components.

2.1.2 For Special Relativity

Definition 4. Tensors and tensor notation

We first define a vector $v \in V$ as an n -dimensional object with a magnitude and direction, defined by n orthogonal components \vec{e}_i , such that

$$\vec{v} = \sum_{i=1}^n a^i \vec{e}_i \quad (4)$$

Furthermore we can define a covector $\omega \in V^*$ as a map that takes a vector and outputs a real value:

$$\omega = \sum_{i=1}^n b_i \tilde{e}^i \quad \omega : V \rightarrow \mathbb{R} \quad (5)$$

with the property that $\tilde{e}^i(\vec{e}_j) = \vec{e}_j(\tilde{e}^i) = \delta_j^i$, such that combining (4) and (5) give:

$$\omega(\vec{v}) = \sum_{i=1}^n b_i a^i \in \mathbb{R} \quad (6)$$

From now on we will use the summation convention. We define an (r, s) -tensor T as a map from r -vectors and s -covectors to the real numbers, i.e.

$$T : V \times \dots \times V \times V^* \times \dots \times V^* \rightarrow \mathbb{R} \quad (7)$$

And we define an (r, s) -tensor space as a map from r -vector spaces and s -dual vector spaces to the set of smooth functions:

$$\mathbb{T} : TM \otimes \dots \otimes TM \otimes T^*M \otimes \dots \otimes T^*M \rightarrow C^\infty \quad (8)$$

2.2 Quantum mechanics

In quantum mechanics [Fol08, §3.1] we deal and work with *observables*, which are physical quantities. From a mathematical point of view these observables are usually unbounded operators in Hilbert spaces, as we have introduced in the prior subsection.

Definition 5. [Fol08, §3.2 p.49]

The time evolution of a quantum system is given by a one-parameter group $U(t)$ of unitary maps, with its corresponding observable given by the Hamiltonian H , i.e:

$$U(t) = e^{\frac{tH}{\hbar}} \quad (9)$$

Definition 6. (Classic Schrödinger's equation)

The following differential equation is defined as *Schrödinger's equation* given a potential V

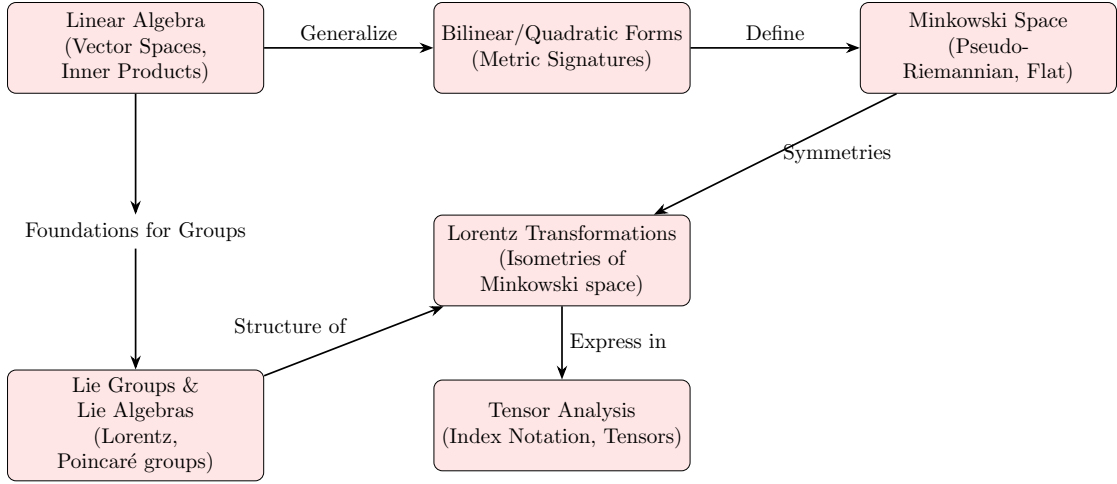


Figure 2: Diagram showcasing the relation between different mathematical concepts used in SR.

(an operator):

$$i\hbar \frac{\partial}{\partial t} f = -\frac{\hbar^2}{2m} \nabla \cdot \nabla f + V f \quad (f(\cdot, t) = U(t)f) \quad (10)$$

Derivation. This arises from transforming the time evolution for Hamiltonian mechanics, that uses Poisson brackets $\{, \}$, into one that uses Lie brackets $[,]$ in the following manner:

$$\{, \cdot \} \rightarrow \frac{1}{i\hbar} [, \cdot]$$

Such that the time evolution becomes:

$$\frac{d}{dt} f = \{f, H\} + \partial_t f \rightarrow \frac{d}{dt} f = \frac{i}{\hbar} [H, f] + \partial_t f$$

This is the equation of motion for the Heisenberg picture, yet Schrödinger and Heisenberg pictures are mathematically equivalent [Fey48] so this is a valid derivation.

2.3 Special relativity

In special relativity we go from Galilean transformation defined on euclidean space to Lorentz transformations defined on Minkowski spacetime.

Definition 7. (Minkowski metric) Define $\eta : V \times V \rightarrow \mathbb{R}$ a rank 2 tensor whose components $\eta_{\alpha\beta}$ are defined by the matrix:

$$(\eta)_{\alpha\beta} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & -1 \end{pmatrix} \quad (11)$$

Definition 8. (Lorentz group)

The Lorentz group is defined as the group of linear maps

$$x^\alpha = \Lambda^\alpha_\beta x^\beta$$

that preserve distances on a Minkowski metric, that is, the line element $ds^2 = \eta_{\alpha\beta} dx^\alpha dx^\beta$ remains unchanged.

3 Quantum Field Theory (QFT)

After Schrödinger developed his successful equation for the quantized Hamiltonian (10), the next goal was to find an equation that connects QM with SR, as (10) did not interpret time and space in the way special relativity does, that is it treats space as an operator and time as a parameter ([Fol08, §4.1]).

Also, in QM, particles are described by wavefunctions that evolve in time. Instead in QFT, particles can be viewed as excitations of fields, which are functions defined across spacetime, and the Klein-Gordon equation is the simplest of such scalar fields.

Around the year 1926, Oscar Klein and Walter Gordon found an expression for an equation that describes a relativistic electron. Erwin Schrödinger and Vladimir Fock also developed this equation by themselves.

Definition 9. Klein-Gordon equation

Let $\square = \eta^{\mu\nu} \partial_\mu \partial_\nu$ be the d'Alembert operator, with $\eta_{\mu\nu} = \text{diag}(1, -1, \dots, -1)$. The Klein-Gordon equation describing the behavior of a 0-spin particle on a free field is:

$$(\square + m^2)\psi = 0 \quad (12)$$

Derivation. [Fol08, §4.1] The most straightforward approach is to consider the relativistic notation for the momentum operator $p^\mu = i\partial^\mu$ and the energy-momentum relation given by $p_\mu p^\mu = m^2$, applying this to a field ϕ we obtain equation (12)

In this relativistic quantum mechanics setting we care about fields ψ such that $\psi \in \mathcal{N}(\square + m^2)$. This is viewed as a constraint such that ψ satisfies the mass-shell condition, i.e it belongs to the allowed physical field configurations for a scalar particle of mass m

Proposition 1. The Klein-Gordon equation (12) is invariant under Lorentz transformations.

Proof. [htt] Define a transformation Λ_ν^μ such that $\Lambda_\alpha^\mu \Lambda_\beta^\nu \eta_{\mu\nu} = \eta_{\alpha\beta}$ and $\Lambda_\alpha^\mu \eta_{\mu\nu} (\Lambda^{-1})^\nu_\beta = \eta_{\alpha\beta}$ from metric commutation. Take the operator \square and transform it (we will forget the indices for sake of notation, but they are summed over):

$$\square' = (\Lambda \Lambda \eta) \Lambda^{-1} \partial \Lambda^{-1} \partial$$

As η and ∂ commute, we obtain:

$$\square' = \Lambda \Lambda \Lambda^{-1} \Lambda^{-1} \eta \partial \partial = \eta \partial \partial = \square$$

Furthermore, $m^2 \in \mathbb{R}$ is trivially invariant, and $\psi'(x') := \psi(x)$. Then:

$$(\square' + m^2)\psi'(x') = (\square + m^2)\psi(x) \quad (13)$$

And the equation is Lorentz invariant. □

Proposition 2. The operator $(\square + m^2)$ is unbounded and symmetric on the Hilbert space \mathcal{H} . Furthermore, given certain domain constraints, it is also self-adjoint.

Proof. First, it is clearly unbounded as differential operators are unbounded. Second, let

$f, g \in C_c^2(\Omega) \subset \mathcal{H}$ and use the inner product on Hilbert spaces (1):

$$\begin{aligned} \langle (\square + m^2)f, g \rangle &= \int_{\Omega} (\square + m^2)f \bar{g} \, dt d^3x \\ &= \int_{\Omega} f (\square + m^2)\bar{g} \, dt d^3x \\ &= \langle f, (\square + m^2)g \rangle \end{aligned}$$

after integration by parts. □

4 Energy identities, existence and uniqueness.

In the field of partial differential equations it is quite common to define a function that states an 'energy' on a system, a functional approach to the notion of physical energies, though sometimes without much meaning of 'energy' per se in a mathematical sense.

Energy estimates can be viewed as positive definite functions that either preserve or decrease their values as they evolve in time. There are quite a few definitions depending on the problem at hand, as it is our goal to deal with the Klein-Gordon equation, we define the following:

Definition 10. (Energy estimates for the Klein-Gordon equation) [Eva10, §12.1.1]

Let $u(x, t)$ be a solution to the Klein-Gordon equation (12), then:

$$E(t) = \int_{\mathbb{R}^3} \frac{1}{2} (u_t^2 + |Du|^2 + m^2 u^2) d^3x \quad (14)$$

is its corresponding energy.

Derivation. Let $\Omega = [0, T] \times \mathbb{R}^3$ and define $I[\cdot]$, representing a functional, as:

$$I[u] = \int_{\Omega} \mathcal{L}(Du, u, x) d^3x dt \quad (15)$$

Let $\mathcal{L}(Du, u, x)$ be a Lagrangian density defined as

$$\mathcal{L}(Du, u, x) = \frac{1}{2} \partial_{\mu} u \partial^{\mu} u + \frac{1}{2} m^2 u^2$$

motivated from the Lagrangian of the classical harmonic oscillator $L = \frac{1}{2} m v^2 - \frac{1}{2} m \omega^2 x^2$. [Atk]

We rewrite the functional (15) as :

$$I[u] = \int_0^T \int_{\mathbb{R}^3} \frac{1}{2} \partial_{\mu} u \partial^{\mu} u + \frac{1}{2} m^2 u^2 d^3x dt$$

And we define (14):

$$E[u](t) = \int_{\mathbb{R}^3} \frac{1}{2} \partial_{\mu} u \partial^{\mu} u + \frac{1}{2} m^2 u^2 d^3x \quad (16)$$

$$= \int_{\mathbb{R}^3} \frac{1}{2} (u_t^2 + |Du|^2 + m^2 u^2) d^3x \quad (17)$$

Proposition 3. Let $g \in C_c^2(\mathbb{R}^3)$, $f \in C_c^1(\mathbb{R}^3)$ be functions with compact support. Then the fol-

lowing initial value problem for the Klein-Gordon equation:

$$\begin{cases} (\square + m^2)\psi(x, t) = 0 & (x, t) \in \Omega \\ \partial_t \psi(x, 0) = f(x) \\ \psi(x, 0) = g(x) \end{cases} \quad (18)$$

Has a unique classical solution $\psi(x, t)$ given by:

$$\psi(x, t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\hat{g}(k) \cos(\omega_k t) + \frac{\hat{f}(k)}{\omega_k} \sin(\omega_k t) \right) e^{-ik \cdot x} d^3 k \quad (19)$$

With $\omega_k = \sqrt{|k|^2 + m^2}$, $m > 0$ and $\hat{g}(k), \hat{f}(k)$ the Fourier transforms of g, f , respectively.

Proof. Uniqueness. Let $\psi_1, \psi_2 \in C^2(\Omega)$ solve (18), define $w = \psi_1 - \psi_2$. Then w solves:

$$\begin{cases} (\square + m^2)w(x, t) = 0 & (x, t) \in \Omega \\ \partial_t w(x, 0) = 0 \\ w(x, 0) = 0 \end{cases} \quad (20)$$

Now using our energy (14) and our initial conditions from (18) we have the following:

$$E(0) = \int_{\mathbb{R}^3} \frac{1}{2} (w_t^2 + |Dw|^2 + m^2 w^2) d^3 x = 0 \quad (21)$$

Let us take its time derivative and integrate by parts the space derivative:

$$\begin{aligned} \frac{d}{dt} E(t) &= \int_{\mathbb{R}^3} (w_t w_{tt} + |Dw| |Dw_t| + m^2 w w_t) d^3 x \\ &= \int_{\mathbb{R}^3} w_t (w_{tt} - \Delta w + m^2 w) d^3 x \\ &= 0 \end{aligned}$$

This in return implies that the energy remains constant throughout time, so:

$$E(t) = \int_{\mathbb{R}^3} \frac{1}{2} (w_t^2 + |Dw|^2 + m^2 w^2) d^3 x = 0, \quad \forall t \in [0, T] \quad (22)$$

Then $w_t = 0$, $Dw = 0$ and so $w = 0$, therefore $\psi_1 = \psi_2$ and our solution is unique.

Existence. We define the Fourier transformation of ψ as follows:

$$\hat{\psi}(k, t) = F[\psi(x, t)] = \int_{\mathbb{R}^3} \psi(x, t) e^{ix \cdot k} d^3 x \quad (23)$$

Such that we transform equation (18) into:

$$F[(\square + m^2)\psi] = 0 \quad \partial_t^2 \hat{\psi} + (|k|^2 + m^2) \hat{\psi} = 0 \quad (24)$$

$$F[\partial_t \psi_0] = \hat{f}(k) \quad \rightarrow \quad \partial_t \hat{\psi}_0 = \hat{f}(k) \quad (25)$$

$$F[\psi_0] = \hat{g}(k) \quad \hat{\psi}_0 = \hat{g}(k) \quad (26)$$

Equation (24) gives us an ODE which we can easily solve:

Define $\omega_k^2 = |k|^2 + m^2$, then:

$$\partial_t^2 \hat{\psi} = -\omega_k^2 \hat{\psi} \quad (27)$$

From this we have the solution

$$\hat{\psi}(k, t) = A \cos(\omega_k t) + B \sin(\omega_k t) \quad (28)$$

Using (25) and (26) we have for A and B :

$$\begin{aligned} \partial_t \hat{\psi}(k, 0) &= -A\omega_k \sin(0) + B\omega_k \cos(0) &\rightarrow & B\omega_k = \hat{f}(k) \\ \hat{\psi}(k, 0) &= A \cos(0) + B \sin(0) &\rightarrow & A = \hat{g}(k) \end{aligned}$$

So $\hat{\psi}$ becomes:

$$\hat{\psi}(k, t) = \hat{g}(k) \cos(\omega_k t) + \frac{\hat{f}(k)}{\omega_k} \sin(\omega_k t) \quad (29)$$

Now we transform back into $\psi(x, t)$:

$$\psi(x, t) = \frac{1}{(2\pi)^3} \int_{\mathbb{R}^3} \left(\hat{g}(k) \cos(\omega_k t) + \frac{\hat{f}(k)}{\omega_k} \sin(\omega_k t) \right) e^{-ik \cdot x} d^3 k \quad (30)$$

As f, g , are compact, bounded function, and $\cos(\omega_k t)$ and $\sin(\omega_k t)$ are bounded, furthermore we assume $m \in \mathbb{R}$ such that $\omega_k > 0, \forall k \in \mathbb{R}^3$, then the integral is well defined and ψ exists. \square

5 Appendix

5.1 Physics

Statement 1. For electromagnetic fields we define the following relations in normal units - from top to bottom: Gauss's law, Gauss's law for magnetism, Faraday's law, Ampere-Maxwell law -:

$$\nabla \cdot \vec{E} = \rho \quad (31)$$

$$\nabla \cdot \vec{B} = 0 \quad (32)$$

$$\nabla \times \vec{E} = -\frac{\partial \vec{B}}{\partial t} \quad (33)$$

$$\nabla \times \vec{B} = \vec{j} + \frac{\partial \vec{E}}{\partial t} \quad (34)$$

Definition 11. (Summation convention) Given an equation with multiple indices, we use the following convention to ease notation:

- Any repeating indices induces a summation over all components
- Any non-repeating indices are called dummy indices, and all sides of the equation must match the dummy indices used.

5.2 Functional analysis

Definition 12. (Banach spaces)

A Banach space X has the following properties:

1. **Normed:** A space is normed if it allows a mapping $\|\cdot\| : X \rightarrow [0, \infty)$ with the properties:
 - $\|u + v\| \leq \|u\| + \|v\|$ for all $u, v \in X$
 - $\|\lambda u\| = |\lambda| \|u\|$ for all $u \in X, \lambda \in \mathbb{R}$
 - $\|u\| = 0 \iff u = 0$
2. **Completeness:** A normed space is called complete if each Cauchy sequence $\{u_k\}_{k=1}^{\infty} \subset X$ converges.

References

- [Fey48] R. P. Feynman. "Space-Time Approach to Non-Relativistic Quantum Mechanics". In: *Reviews of Modern Physics* 20.2 (1948), pp. 367–387. DOI: 10.1103/RevModPhys.20.367. URL: <https://journals.aps.org/rmp/pdf/10.1103/RevModPhys.20.367>.
- [Bla06] Bruce Blackadar. *Operator Algebras: Theory of C^* -Algebras and von Neumann Algebras*. Vol. 122. Encyclopaedia of Mathematical Sciences. Berlin, Heidelberg: Springer, 2006. ISBN: 3-540-28486-9.
- [Fol08] Gerald B. Folland. *Quantum Field Theory: A Tourist Guide for Mathematicians*. Vol. 149. Mathematical Surveys and Monographs. Providence, RI: American Mathematical Society, 2008. ISBN: 978-0-8218-4373-4.

- [Eva10] Lawrence C. Evans. *Partial Differential Equations*. 2nd ed. Vol. 19. Graduate Studies in Mathematics. Providence, RI: American Mathematical Society, 2010. ISBN: 978-0-8218-4974-3. DOI: 10.1090/gsm/019.
- [Sch12] Konrad Schmüdgen. *Unbounded Self-Adjoint Operators on Hilbert Space*. Vol. 265. Graduate Texts in Mathematics. Springer, 2012. ISBN: 978-94-007-4753-1. DOI: 10.1007/978-94-007-4753-1.
- [Cho15] Yvonne Choquet-Bruhat. *Introduction to General Relativity, Black Holes, and Cosmology*. Oxford: Oxford University Press, 2015. ISBN: 978-0-19-966645-4. URL: <https://global.oup.com/academic/product/introduction-to-general-relativity-black-holes-and-cosmology-9780199666461>.
- [htt] gented (<https://physics.stackexchange.com/users/84488/gented>). *How can I prove that d'Alembert operator is invariant under Lorentz transformations?* Physics Stack Exchange. URL: <https://physics.stackexchange.com/q/223568> (version: 2017-04-13). eprint: <https://physics.stackexchange.com/q/223568>. URL: <https://physics.stackexchange.com/q/223568>.
- [Atk] Jeremy Atkins. *The Free Klein-Gordon Field Theory*. https://www.sas.rochester.edu/pas/assets/pdf/undergraduate/the_free_klein_gordon_field_theory.pdf. Department of Physics and Astronomy, University of Rochester.