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An Analysis on Exact Solution of Klein–Gordon Equation: A Relativistic Version of the Schrodinger Equation

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Abstract – In the present paper is to understand and compare various numerical methods for solving the nonlinear Klein–Gordon (KG) equation. The nonlinear KG equation might be viewed as the most simplest form of the charged klein-gordon field. We derive exact analysis about physical problems of the Klein-Gordon equation and to introduce electromagnetic interactions into the KG equation.

INTRODUCTION

The Klein-Gordon equation (or Klein-Fock-Gordon equation) is a relativistic version of the Schrodinger equation, which describes scalar (or pseudoscalar) spinless particles. The Klein-Gordon equation was actually first found by Schrodinger, before he made the discovery of the equation that now bears his name. He rejected it because he couldn't make it fit the data (the equation doesn't take into account the spin of the electron); the way he found his equation was by making simplification in the Klein-Gordon equation. Later, it was revived and it has become commonly accepted that Klein-Gordon equation is the appropriate model to describe the wave function of the particle that is charge-neutral, spinless and relativistic effects can't be ignored.

It has important applications in plasma physics, together with Zakharov equation describing the interaction of Langmuir wave and the ion acoustic wave in a plasma, in astrophysics together with Maxwell equation describing a minimally coupled charged boson field to a spherically symmetric space time, in biophysics together with another Klein-Gordon equation describing the long wave limit of a lattice model for one-dimensional nonlinear wave processes in a bi-layer and so on. Furthermore, Klein-Gordon equation coupled with Schrodinger equation (Klein-Gordon-Schrodinger equations or KGS) is introduced in and it describes a system of conserved scalar nucleons interacting with neutral scalar mesons coupled through the Yukawa interaction. As is well known, KGS is not exactly integrable, so the numerical study on it is very important.

Derivation of the Klein-Gordon equation-This chapter is devoted to derive the Klein-Gordon equation. From elementary quantum mechanics, we know that the Schrodinger equation for free particle is

$$i\hbar \frac{\partial}{\partial t} \phi = \frac{\mathbf{P}^2}{2m} \phi, \quad (1)$$

where ϕ is the wave function, m is the mass of the particle, $\hbar$ is Planck's constant, and $\mathbf{P} = -i\hbar \nabla$ is the momentum operator.

The Schrodinger equation suffers from not being relativistically covariant, meaning that it does not take into account Einstein's special relativity. It is natural to try to use the identity from special relativity

$$E = \sqrt{\mathbf{P}^2 c^2 + m^2 c^4} \phi, \quad (2)$$

for the energy (c is the speed of light); then, plugging into the quantum mechanical momentum operator, yields the equation

$$i\hbar \frac{\partial}{\partial t} \phi = \sqrt{(-i\hbar \nabla)^2 c^2 + m^2 c^4} \phi. \quad (3)$$

This, however, is a cumbersome expression to work with because of the square root. In addition, this equation, as it stands, is nonlocal. Klein and Gordon instead worked with more general square of this

equation (the Klein-Gordon equation for a free particle), which in covariant notation reads

$$(\square^2 + \mu^2)\phi = 0, \quad (4)$$

where $\mu = \frac{mc}{\hbar}$ and $\square^2 = \frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \nabla^2$. This operator ($\square^2$) is called as the d'Alembert operator. This wave equation (4) is called as the Klein-Gordon equation. It was in the middle 1920's by E. Schrodinger, as well as by O. Klein and W. Gordon, as a candidate for the relativistic analog of the nonrelativistic Schrodinger equation for a free particle.

In order to obtain a dimensionless form of the Klein-Gordon equation (4), we define the normalized variables

$$\tilde{t} = \mu c t, \quad \tilde{x} = \mu x. \quad (5)$$

Then plugging (3.5) into (3.4) and omitting all $\sim$, we get the following dimensionless standard Klein-Gordon equation

$$\partial_{tt}\phi - \Delta\phi + \phi = 0. \quad (6)$$

For more general case, we consider the nonlinear Klein-Gordon equation

$$\partial_{tt}\phi - \Delta\phi + F(\phi) = 0, \quad (7)$$

where $G(\phi) = \int_0^\phi F(\phi) d\phi$.

Numerical methods for the Klein-Gordon equation

- In this chapter, we review some existing numerical methods for the nonlinear Klein-Gordon equation and present a new method for it. For simplicity of notation, we shall introduce the methods in one spatial dimension ($d = 1$). Generalization to $d > 1$ is straightforward by tensor product grids and the results remain valid without modification. For $d = 1$, the problem becomes

$$\partial_{tt}\phi - \partial_{xx}\phi + F_{\text{lin}}(\phi) + F_{\text{non}}(\phi) = 0, \quad a < x < b, \quad t > 0, \quad (8)$$

$$\phi(a, t) = \phi(b, t), \quad \partial_x \phi(a, t) = \partial_x \phi(b, t), \quad t \geq 0, \quad (9)$$

$$\phi(x, 0) = \phi^{(0)}(x), \quad \partial_t \phi(x, 0) = \phi^{(1)}(x), \quad a \leq x \leq b, \quad t \geq 0, \quad (10)$$

where $F_{\text{lin}}(\phi)$ represents the linear part of $F(\phi)$ and $F_{\text{non}}(\phi)$ represents the nonlinear part of it. As it is known in this Section, the KG equation has the properties

$$H(t) = \int_a^b \left[\frac{1}{2} \phi_t(x, t)^2 + \frac{1}{2} \phi_x(x, t)^2 + G(\phi) \right] dx = H(0), \quad (11)$$

$$P(t) = \int_a^b [\phi_t(x, t) \phi_x(x, t)] dx = P(0), \quad (12)$$

$$A(t) = \int_a^b \left[x \left(\frac{1}{2} \phi_t(x, t)^2 + \frac{1}{2} \phi_x(x, t)^2 + G(\phi) \phi_t(x, t) \right) + t \phi_t(x, t) \phi_x(x, t) \right] dx = A(0). \quad (13)$$

In some cases, the boundary condition (3.9) may be replaced by

$$\phi(a, t) = \phi(b, t) = 0, \quad t \geq 0. \quad (14)$$

We choose the spatial mesh size $h = \Delta x > 0$ with $h = (b - a)/M$ for M being an even positive integer, the time step being $k = \Delta t > 0$ and let the grid points and the time step be

$$x_j := a + jh, \quad j = 0, 1, \dots, M; \\ t_m := mk, \quad m = 0, 1, 2, \dots. \quad (15)$$

Let ϕ_j^m be the approximation of $\phi(x_j, t_m)$. Existing numerical methods - There are several numerical methods proposed in the literature for discretizing the nonlinear Klein-Gordon equation. We will review these numerical schemes for it. The schemes are the following

A). This is the simplest scheme for the nonlinear Klein-Gordon equation and has had wide use :

$$\frac{\phi_j^{n+1} - 2\phi_j^n + \phi_j^{n-1}}{k^2} - \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{h^2} + F(\phi_j^n) = 0, \\ j = 0, \dots, M-1, \quad (16)$$

$$\phi_M^{n+1} = \phi_0^{n+1}, \quad \phi_{-1}^{n+1} = \phi_{M-1}^{n+1}. \quad (17)$$

The initial conditions are discretized as

$$\phi_j^0 = \phi^{(0)}(x_j), \quad \frac{\phi_j^1 - \phi_j^{-1}}{2k} = \phi^{(1)}(x_j), \quad 0 \leq j \leq M-1. \quad (18)$$

B). This scheme was proposed by Ablowitz, Kruskal, and Laclik :

$$\frac{\phi_j^{n+1} - 2\phi_j^n + \phi_j^{n-1}}{k^2} - \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{h^2} + F\left(\frac{\phi_{j+1}^n + \phi_{j-1}^n}{2}\right) = 0, \\ j = 0, \dots, M-1, \quad (19)$$

$$\phi_M^{n+1} = \phi_0^{n+1}, \quad \phi_{-1}^{n+1} = \phi_{M-1}^{n+1}. \quad (20)$$

The initial conditions are discretized as

$$\phi_j^0 = \phi^{(0)}(x_j), \quad \frac{\phi_j^1 - \phi_j^{-1}}{2k} = \phi^{(1)}(x_j), \quad 0 \leq j \leq M-1. \quad (21)$$

C). This scheme has been studied by Jimenez :

$$\frac{\phi_j^{n+1} - 2\phi_j^n + \phi_j^{n-1}}{k^2} - \frac{\phi_{j+1}^n - 2\phi_j^n + \phi_{j-1}^n}{h^2} + \frac{G(\phi_{j+1}^n) - G(\phi_{j-1}^n)}{\phi_{j+1}^n - \phi_{j-1}^n} = 0, \quad j = 0, \dots, M-1, \quad (22)$$

$$\phi_M^{n+1} = \phi_0^{n+1}, \quad \phi_{-1}^{n+1} = \phi_{M-1}^{n+1}. \quad (23)$$

The initial conditions are discretized as

$$\phi_j^0 = \phi^{(0)}(x_j), \quad \frac{\phi_j^1 - \phi_j^{-1}}{2k} = \phi^{(1)}(x_j), \quad 0 \leq j \leq M-1. \quad (24)$$

The existing numerical methods are of second-order accuracy in space and second-order accuracy in time. Our new method shown in the next section is of spectral-order accuracy in space, which is much more accurate than them.

Our new numerical method - We discretize the Klein-Gordon equation by using a pseudospectral method for spatial derivatives, followed by application of a Crank-Nicolson/leap-frog method for linear/nonlinear terms for time derivative.

$$\frac{\phi_j^{m+1} - 2\phi_j^m + \phi_j^{m-1}}{k^2} - D_{xx}^f [\beta \phi_j^{m+1} + (1-2\beta)\phi_j^m + \beta \phi_j^{m-1}] + F_{lin}(\beta \phi_j^{m+1} + (1-2\beta)\phi_j^m + \beta \phi_j^{m-1}) + F_{non}(\phi_j^m) = 0 \quad j = 0, \dots, M, \quad m = 1, 2, \dots \quad (25)$$

Where $0 \leq \beta \leq 1/2$ is a constant; D_{xx}^f a spectral differential operator approximation of ∂_{xx} , is defined as

$$D_{xx}^f U|_{x=x_j} = - \sum_{l=-M/2}^{M/2-1} \mu_l^2 (\tilde{U})_l e^{i\mu_l(x_j-a)}, \quad (26)$$

where $(\tilde{U})_l$ the Fourier coefficient of a vector $U = (U_0, U_1, U_2, \dots, U_M)^T$ with $U_0 = U_M$, is defined as

$$(\tilde{U})_l = \frac{1}{M} \sum_{j=0}^{M-1} U_j e^{-i\mu_l(x_j-a)}, \quad \mu_l = \frac{2\pi l}{b-a}, \quad l = -\frac{M}{2}, \dots, \frac{M}{2} - 1. \quad (27)$$

The initial condition are discretized as

$$\phi_j^0 = \phi^0(x_j), \quad \frac{\phi_j^1 - \phi_j^{-1}}{2k} = \phi^{(1)}, \quad j = 0, 1, 2, \dots, M-1. \quad (28)$$

PHYSICAL PROBLEMS OF THE KLEIN-GORDON EQUATION

The Klein-Gordon equation fulfills the laws of special relativity, but contains two fundamental problems, which have to be taken care of for the equation to be physically meaningful.

The first problem becomes obvious when considering the solutions of the different equations. Using the ansatz

$$\begin{aligned} \psi(x) &= a e^{i(\vec{k} \cdot \vec{r} - \omega t)} \\ &= a e^{-ik_\mu x^\mu} \end{aligned} \quad (29)$$

with

$$k_\mu = \begin{pmatrix} \frac{w}{c} \\ -\vec{k} \end{pmatrix} \quad (30)$$

One obtains

$$a \left[-k_\mu k^\mu + \left(\frac{mc}{\hbar} \right)^2 \right] = 0 \quad (31)$$

$$k^2 = k_\mu k^\mu = \left(\frac{mc}{\hbar} \right)^2 \quad (32)$$

from which follows

$$\begin{aligned} (k^0)^2 &= \vec{k}^2 + \left(\frac{mc}{\hbar} \right)^2 \\ k^0 &= \pm \sqrt{\vec{k}^2 + \left(\frac{mc}{\hbar} \right)^2} \end{aligned} \quad (33)$$

This means that the Klein-Gordon equation allows negative energies as solution. Formally, one can see

that the information about the sign is lost. However, all solutions have to be considered, and there is the problem of the physical interpretation of negative energies.

The second problem with the Klein-Gordon equation is less obvious. It occurs when interpreting the function $\psi(x)$ as probability amplitude. Interpretation of $\psi(x)$ as probability amplitude is only possible if there exists a probability density $\rho(x)$ and a current $\vec{j}(x)$ that fulfill a continuity equation

$$\frac{\partial}{\partial t} \rho + \vec{\nabla} \cdot \vec{j} = 0, \quad (34)$$

which guarantees that no "probability" is lost.

Since we deal with a covariant equation, we define

$$\begin{aligned} j^0(x) &:= c\rho(x) \\ j^\mu(x) &:= \begin{pmatrix} j^0(x) \\ \vec{j}(x) \end{pmatrix} \end{aligned} \quad (35)$$

and obtain the covariant form

$$\frac{\partial}{\partial x^\mu} j^\mu = \partial_\mu j^\mu = 0. \quad (36)$$

Eqs. (34 and (35) correspond in form and content the charge conservation in electrodynamics.

Non-relativistic ally one has

$$\begin{aligned} \rho_{NR} &= \psi^* \psi \\ \vec{j}_{NR} &= \frac{\hbar}{(2mi)} [\psi^* \vec{\nabla} \psi] \end{aligned} \quad (37)$$

and thus one expects in the relativistic case also bilinear expressions in ψ for ρ and $\vec{j}$. If one defines a density ρ according to (37) with the solution (29), it is easy to show that, this density does not fulfill a continuity equation. This has to be expected since j^μ has to be a four-vector so that (35) is valid in all Lorentz systems. Thus, it is obvious to generalize (37) to

$$j^\mu := \frac{i\hbar}{2m} \psi^* \overleftrightarrow{\partial}^\mu \psi \quad (38)$$

where

$$A^* \overleftrightarrow{\partial}^\mu B := A^* (\partial^\mu B) - (\partial^\mu A^*) B. \quad (39)$$

Consider

$$\begin{aligned} \partial_\mu j^\mu &= \frac{i\hbar}{2m} \partial_\mu (\psi^* \overleftrightarrow{\partial}^\mu \psi) \\ &= \frac{i\hbar}{2m} [(\partial_\mu \psi^*)(\partial^\mu \psi) + \psi^*(\partial_\mu \partial^\mu \psi) - (\partial_\mu \partial^\mu \psi^*)\psi - (\partial^\mu \psi^*)(\partial_\mu \psi)] \\ &= \frac{i\hbar}{2m} [\psi^*(\square\psi) - (\square\psi^*)\psi] \end{aligned} \quad (40)$$

If ψ fulfills the Klein-Gordon equation, the right-hand side of (40) vanishes, and the continuity equation (35) holds. However, the four-vector defined in (38) contains the second problem:

$$\begin{aligned} \rho &= \frac{1}{c} j^0 \\ &= \frac{i\hbar}{2mc} \psi^* \overleftrightarrow{\partial}^0 \psi \\ &= \frac{i\hbar}{2mc^2} \left[\psi^* \frac{\partial}{\partial t} \psi - \frac{\partial \psi^*}{\partial t} \psi \right] \end{aligned} \quad (41)$$

can be positive or negative, depending on the values of ψ and Since the Klein-Gordon equation denotes a partial differential equation (2nd order) of hyperbolic type, one has the option to arbitrarily choose the functions

$$\psi(\vec{x}, t = 0) \quad \text{and} \quad \frac{\partial}{\partial t} \psi(\vec{x}, t = 0) \quad (42)$$

at the starting time ($t = 0$), and thus obtain, e.g., negative values for $\rho(\vec{x}, t = 0)$. An interpretation of ρ as probability density would mean that the theory allows negative probabilities. This is the problem of the indefinite probability density.

THE CHARGED KLEIN-GORDON FIELD

In case of a complex, i.e. charged scalar field, the current is given with $\partial j^\mu / \partial x^\mu = 0$ and a total charge

$$Q = \frac{ie\hbar}{2mc^2} \int d^3x \left(\varphi^* \frac{\partial \varphi}{\partial t} - \varphi \frac{\partial \varphi^*}{\partial t} \right). \quad (43)$$

To examine charged fields in some more detail, we decompose $\varphi(x)$ into real and imaginary components

$$\varphi(x) = \frac{1}{\sqrt{2}} (\varphi_1(x) + i\varphi_2(x)), \quad (44)$$

where $\varphi_1(x)$ and $\varphi_2(x)$ are real. If $\varphi(x)$ fulfills the Klein-Gordon equation, so do the components $\varphi_1(x)$ and $\varphi_2(x)$

Conversely, the following is true: If two fields $\varphi_1(x)$ and $\varphi_2(x)$ separately fulfill a Klein-Gordon equation with the same mass $m = m_1 = m_2$, then the equations can be replaced by one equation for a complex field, i.e.

With

$$\begin{aligned}\varphi &= \frac{1}{\sqrt{2}}(\varphi_1 + i\varphi_2) \\ \varphi^* &= \frac{1}{\sqrt{2}}(\varphi_1 - i\varphi_2)\end{aligned}\quad (45)$$

$$\begin{aligned}\left(\square + \frac{m^2 c^2}{\hbar^2}\right)\varphi &= 0 \\ \left(\square + \frac{m^2 c^2}{\hbar^2}\right)\varphi^* &= 0\end{aligned}\quad (46)$$

By interchanging φ and φ^* , we obtain the opposite charge. Hence φ and φ^* chamctmzti opposite charges. These studies can. e.g., be applied to the pion triplet (π^+, π^-, π^0)

KLEIN-GORDON EQUATION WITH INTERACTION

To introduce electromagnetic interactions into the KG equation, we use the socalled 'minimal substitution', known from EM

$$p^\mu \rightarrow p^\mu - eA^\mu \quad (47)$$

where A^μ is a four-vector potential. Inserting this into the KG equation gives

$$\left[-\left(i\frac{\partial}{\partial x^\mu} - eA_\mu\right)\left(i\frac{\partial}{\partial x_\mu} - eA^\mu\right) + m^2\right]\Psi(x) = 0 \quad (48)$$

$$\left[\partial_\mu \partial^\mu + m^2 + U(x)\right]\Psi(x) = 0, \quad (49)$$

where the generalized potential $U(x)$ consists of a scalar and vector part

$$\begin{aligned}U(x) &= ie\frac{\partial}{\partial x^\mu}A^\mu + ieA^\mu\frac{\partial}{\partial x^\mu} - e^2A^\mu A_\mu \\ &= i\frac{\partial}{\partial x^\mu}V^\mu + iV^\mu\frac{\partial}{\partial x^\mu} + S\end{aligned}\quad (50)$$

Note that the symmetrized form of the vector terms is required in order to maintain the hermicity of the interaction. In the most general case, the scalar, S ,

and vector, V^μ , parts of the potential can be independent interactions. For the electromagnetic case they are related by

$$\begin{aligned}S &= e^2A^\mu A_\mu \\ V^\mu &= eA^\mu\end{aligned}\quad (51)$$

Using the 'standard' form of $A^\mu \equiv (\Phi, \mathbf{A})$, the KG equation can be written as

$$\left(i\frac{\partial}{\partial t} - e\Phi\right)^2\Psi(\mathbf{x}, t) = \left[(-i\nabla - e\mathbf{A})^2 + m^2\right]\Psi(\mathbf{x}, t) \quad (52)$$

Substituting the positive and negative energy solutions into (52) gives

$$(E_p \mp e\Phi)^2\Psi^{(\pm)}(\mathbf{x}, t) = \left[(\hat{p} \mp e\mathbf{A})^2 + m^2\right]\Psi^{(\pm)}(\mathbf{x}, t) \quad (53)$$

Again, once can use (53) as starting point and use it with more general potentials V and A . For example, let $A = 0$ and $V = e\Phi$, i.e. allow only a scalar potential V . Then

(53) gives

$$(E^2 + V^2 - 2EV)\Psi = (\hat{p}^2 + m^2)\Psi \quad (54)$$

Substituting the relation $E^2 = k^2 + m^2$ between energy and wave vector and using $\hat{p} \rightarrow -i\nabla$ leads to

$$(\nabla^2 + k^2)\Psi = (2EV - V^2)\Psi, \quad (55)$$

which looks like a Schrodinger equation with the equivalent energy dependent potential

$$V^{SE} = \frac{2EV - V^2}{2m} \quad (56)$$

Another type of potential to consider is the Lorentz scalar, which adds to the mass, since

$p^\mu p_\mu = m^2$. The KG equation with coupling to the scalar potential is

$$E^2 \Psi = [\hat{p}^2 + (m + S)^2] \Psi \quad (57)$$

CONCLUSION

It should be stated that this work does not deny the usage of the KG equation as a phenomenological equation. Indeed, by definition, a phenomenological equation is evaluated mainly by its usefulness in describing a specific set of data. This kind of evaluation is of a practical nature and is immune to theoretical counter-arguments.

We discuss the implications of our approach for free real scalar fields offering a direct proof of the uniqueness of the relativistic ally invariant positive-definite inner product on the space of real Klein-Gordon fields.

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