Numerical Methods in Quantum Field Theories

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1 Abstract

In this paper, preliminary results from investigation into the formalism of Quantum Field Theory as well as various numerical techniques used to approximate theoretical models will be presented. First, the two equations of primary interest, the Klein Gordon and Dirac equations, will be introduced and examined for underlying mathematical and physical structure. In the next section, a naive approach to transforming the differential equations into difference equations will be used and their limitations will be discussed. We will then proceed to investigate methods of preserving discrete forms of the continuous symmetries these equations hold. Finally we will discuss how these methods can be combined together in ways that can balance the need for numerical methods to both well approximate the system as well as preserve the symmetry of the equations.

2 Introduction

The formulation of Quantum Field Theory succeeded in unifying Quantum Mechanics with Special Relativity in a very satisfying way. While the subject is nowhere near complete, the interactions described with QFT explain observed behavior so naturally it is impossible to deny its computational ability. However, while the theory allows us to write down very elegant descriptions of how particles with internal degrees of freedom (spin) interact with each other through the Strong, Weak and Electromagnetic Forces, the process of actually calculating values that are physically observable becomes complicated very quickly because the corresponding integrals have no closed form solution. The physicist must truncate an infinite series at some point to begin making a calculation. These approximations can be carried out to arbitrary precision, but this is not the only issue. Ignoring the common divergences that physicists encounter in these approximations, there is the
issue of practicality. It does not make sense to carry out these calculations by hand when a computer can do them exponentially faster. However, a very large sacrifice is made when computation is left to a computer because it only has the ability to add and multiply. Binary cannot represent $\frac{1}{10}$ without truncating an infinite sequence, so the reduction of a very complex integral equation to a series of arithmetic operations is not a trivial process.

3 Klein-Gordon and Dirac Equations

We begin by stating the two primary field equations of interest$^1$.

**Definition 1** (Klein-Gordon Field). Let $\phi(x) = \phi(\vec{x}, t)$ be a real valued scalar field satisfying the Lagrangian density

$$\mathcal{L} = \frac{1}{2}(\partial_{\mu}\phi)^2 - \frac{1}{2}m^2\phi^2$$

Then $\phi$ is called the Klein-Gordon field satisfying the Euler-Lagrange equation

$$\partial^{\mu}\partial_{\mu}\phi + m^2\phi = 0$$

This will be our first relativistic wave equation to consider. As a scalar field it describes the motion of a neutral spin 0 particle who is it’s own antiparticle. If we were to modify it to be complex valued the real and imaginary parts would correspond to a particle-antiparticle pair with opposite

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$^1$Throughout the text the metric signature (+,-,-,-) will be used. Also $\hbar = c = 1$
charges.

Before defining the next field of interest, we define a mathematical object vital to working with the field.

**Definition 2** (Lorentz Algebra). Let $\gamma^\mu$ be $4 \times n$ matrices satisfying the anti-commutation relations

$$\{\gamma^\mu, \gamma^\nu\} = 2g^{\mu\nu} \times 1_n$$

Then we have an $n$-dimensional representation of the Lorentz algebra given by these four matrices from the commutation relations

$$S^\mu{}^\nu = \frac{i}{4}[\gamma^\mu, \gamma^\nu]$$

The elements of the Lorentz algebra satisfy the following commutation relations

$$[S^\mu{}^\nu, S^\rho{}^\sigma] = i(g^{\rho\rho} S^\mu{}^\sigma - g^{\mu\rho} S^\nu{}^\sigma - g^{\nu\sigma} S^\mu{}^\rho + g^{\mu\sigma} S^\nu{}^\rho)$$

In the case of $n = 4$, the $\gamma^\mu$ matrices are the Dirac matrices. Their particular representation will be specified later. With these in mind, we proceed to the next field under consideration.

**Definition 3** (Dirac Field). Let $\psi$ be a 4 component field that transforms under boosts and rotations according to the Lorentz algebra (called a Dirac spinor). Let $\psi$ satisfy:

$$(i\gamma^\mu \partial_\mu - m)\psi(x) = 0$$
This is the Dirac equation. To describe the Lagrangian of the Dirac Field, first define:

$$\bar{\psi} \equiv \psi^\dagger \gamma^0$$

the so called Dirac adjoint. With this, the Lorentz invariant Dirac Lagrangian is

$$\mathcal{L}_{\text{Dirac}} = \bar{\psi}(i\gamma^\mu \partial_\mu - m)\psi$$

This field describes a spin 1/2 particle and its corresponding antiparticle. A solution to the Dirac Field equation is automatically a solution to the Klein-Gordon equation, but not vice versa.

These two fields give us the foundational tools to describe the interactions of relativistic quantum systems. It should be noted that both equations have solutions with negative energies, which was initially seen as a weakness of the theories. Reinterpretation of those solutions as particles corresponding antiparticle resolved those issues. Of course, it is inaccurate to say these two fields describe particles at all, because we have not quantized them yet.

When the quantization procedure is carried out, care must be taken to apply appropriate commutation relations. Specifically, for the Dirac Field we must impose anti-commutation relations to preserve causality and to explain the negative energy solutions in terms of antiparticles.

One final thing to make note of with these equations is the conserved energy norm. Because solutions to the Dirac equation are automatically solutions to the Klein-Gordon equation, it is sufficient to just show the conserved norm
for the Klein-Gordon equation. To do this, we define a quantity called the energy
\[
E(t) = \int_{\mathbb{R}^n} \left| \frac{\partial \phi}{\partial t} \right|^2 + \left| \frac{\partial \phi}{\partial x_1} \right|^2 + \left| \frac{\partial \phi}{\partial x_2} \right|^2 + \cdots + \left| \frac{\partial \phi}{\partial x_n} \right|^2 \, dx
\]
And for our solution \( \phi(\vec{x},t) \), the energy should be conserved (i.e. \( E(t) = E(0) \ \forall \ t \)). This quantity is important in its own right, because it allows us to define a topology on the space of solutions to the Klein-Gordon equation. Any approximation should then have a discrete conserved energy norm in order to recover the structure of the continuous solution.

4 2nd Order Finite Difference Method - A Careless Attempt

To begin, we consider the Klein-Gordon equation in (1+1) dimensions:
\[
(\partial_t^2 - \partial_x^2)\phi(x,t) + \phi(x,t) = 0
\]
There are several conditions that we must impose to effectively translate this differential equation to a difference equation. The first is that we must restrict the equation to some finite region. For simplicity, we will consider a box of side length \( L \) and partition it into \( n \) equal sized intervals. In other words, \( \Delta t = \Delta x = L/n = h \). Additionally, boundary conditions must be specified so that the value of the field is known along the \( x = -h \) and \( x = L + h \) lines. Again, we strive for simplicity and make the field equal to zero everywhere
outside of the box. Finally, we specify an initial condition \( \phi(x, 0) = f(x) \).

With these conditions it is quite simple to formulate a discrete approximation to our field. To evaluate the \( n+1 \)-th time step at the \( k \)-th spacial step:

\[
\phi(kh, (n+1)h) = (\phi((k+1)h, nh) + \phi((k-1)h, nh)(1-h^2/2)) - \phi(kh, (n-1)h)
\]

This difference equation came out nicely because we assumed the step size for the time and spacial steps were equal. In general, we also need to know the value at the \( k \)-th and \( n \)-th step as well. This formulation’s error is second order in both time and space, so by taking smaller step sizes, the error decreases quadratically.

However, there is a glaring issue with this approach, we treated the equation classically and non-relativistically. Even for the simple case of the Klein-Gordon Field, we must affix harmonic oscillators at every point in space. By specifying a finite region, we ensured that our eigenfunctions would have a discrete spectrum, but we did nothing to ensure these eigenfunctions satisfy relativistic constraints, nor did we consider the fact that there is a countably infinite basis of eigenfunctions. We also failed to treat \( \phi(x, t) \) as an operator. It should be obvious then that more care is needed to apply numerical methods for quantum fields.
5 A Second Attempt

From the last section, it is now obvious that the equation of motion of a field is not the correct thing to consider. This is obvious when the importance of the Lagrangian in Quantum Field Theory is recognized. We are ultimately interested in describing interactions among particles and calculating scattering cross sections and probability amplitudes. To return to the Klein-Gordon equation, let’s consider the true form of our field:

\[
\phi(\vec{x}, t) = \int \frac{d^3p}{(2\pi)^3} \frac{1}{\sqrt{2E_\vec{p}}} (a_\vec{p}e^{-ip^\mu x^\mu} + a_\vec{p}^\dagger e^{ip^\mu x^\mu})
\]

From here it is obvious that \( \phi \) should act on state kets. If we want to calculate the amplitude for a particle to propagate between two points we must evaluate:

\[
D(x - y) = \langle 0 | \phi(x) \phi(y) | 0 \rangle = \int \frac{d^3p}{(2\pi)^3} \frac{1}{\sqrt{2E_\vec{p}}} e^{-ip^\mu (x^\mu - y^\mu)}
\]

We now begin to touch on the heart of the matter. Calculations in Quantum Field Theory are not differential equations, they are integral equations. Attempting to apply numerical techniques to the equations of motion for the Klein-Gordon and Dirac fields will give solutions that are difficult to interpret and possibly nonphysical and probably nonsense.
6 A Solution and Applications

We have avoided the functional integral until now, because it is not the most obvious approach. Of course, by prioritizing the Lagrangian over the Hamiltonian, we move away from the more familiar grounds of Quantum Mechanics, and so the picture becomes less algebraic and more analytic. However, it is undeniable that the path integral formulation makes concerns about preserving symmetry and Lorentz invariance much less of an issue. The reason this method was not considered from the start stems from a numerical standpoint. Solving an integral equation is more involved than a differential equation and is substantially more computationally intensive. This approach does allow for many different techniques to be applied and allows us to delay the need to discretized any equations, or at least to work with semi-discrete equations. Additionally, by working with integral equations we no longer work with point by point evaluation, but with the construction of explicit functions that both well approximate the equation and are easier to work with. In short, this approach trades ease of computation for flexibility.

The flexibility of integral equations comes from the two radically different methods of evaluating the integral. Using the power of Stoke’s Theorem, we can change the type of integral from surface to volume or vice versa, depending on the nature of the integrand. We could also construct a weak solution using functional analysis. This variational method has been successfully applied to Atomic Physics and could be quite useful for examining the bound
states of elementary particles.

7 Conclusion

This paper represents the preliminary investigations into how systems in Quantum Field Theory can be numerically evaluated. It is evident that the restrictions quantization and relativity put on the equations make a consistent and accurate numerical approach complex. Further investigation will be made into how successfully numerical schemes can be constructed for the path integral formulation of Quantum Field Theory. In doing so, methods of transforming continuous symmetries into discrete ones will be explored to see if the approximations made for the integral equations retain any sort of symmetry.
References:


M. Peskin and D. Schroeder, An Introduction to Quantum Field Theory (Westview Press, 1995).


J.J. Sakurai and S.F Tuan, Modern Quantum Mechanics (Addison-Wesley, 1994).