A New Approach to Numerical Quantum Field Theory

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Abstract

In this note we present a new numerical method for solving Lattice Quantum Field Theory. This Source Galerkin Method is fundamentally different in concept and application from Monte Carlo based methods which have been the primary mode of numerical solution in Quantum Field Theory. Source Galerkin is not probabilistic and treats fermions and bosons in an equivalent manner.

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1 Introduction

Over a decade ago, it was realized that the algorithms and computer power existed to calculate non-perturbative consequences of Quantum Field Theory \([1]\). Initial results using Monte Carlo methods and the quenched approximation were a striking confirmation of the power of numerical methods and the general correctness of the ideas of lattice QCD \([2]\). After countless hours of calculation with ever more powerful computers and vast improvements of the initial class of algorithms, there is still the hope of great success as machines become much faster. While there has been demonstrable progress, it can be argued that important but mostly incremental improvements in results have been made.

It is the purpose of this note to introduce a very different class of approaches to numerical quantum field theory. The new methods, while not without their own difficulties, have the promise of allowing a great increase in the accuracy and speed of numerical calculation. Particularly important is that fermions can be treated in essentially the same manner as bosons.

For clarity, we will illustrate these ideas with very simple examples. Our initial analysis was produced through the use of ALJABR* (a product of Fort Pond Research) which is a very reliable computer algebra program. It is not necessary to resort to Fortran or C coded implementations of our methods until quite complicated systems are studied. A good workstation will produce a remarkable number of results.

Our approach is based on considering field theory in the presence of external sources. We start with the functional equations for the vacuum amplitude \(Z\). On a lattice, these are converted to a set of coupled linear differential equations in the discretized sources \(J\).

The high degree of symmetry due to the translation and reflection invariance of the lattice can be used to our advantage in constructing the solution. For this note, \(Z\) will be approximated by a power series in \(J\). Faster convergence and the full power of our ideas is obtained with other more structured approximations that will be presented elsewhere.

Truncated approximations in multiple dimensions are intrinsically inconsistent. One particularly elegant method to handle this problem is to require that weighted averages of the equation residual vanish. A clever choice of weight functions speeds the convergence to the exact solution. Techniques of this sort are familiar in the numerical solution of differential equations and are called Galerkin methods \([3]\). The accuracy of the approximation can be judged by measuring its numerical stability and convergence.
Since our expansion and weight functions depend on the external sources, we call this method the Source Galerkin method. Except for the anti-commutation of fermionic sources, fermions and bosons can be treated symmetrically. Nested solutions for dynamical fermion problems become possible with existing computers.

2 Functional Formulation in the Presence of Sources

We begin by studying a scalar field $\Phi(x)$ in the presence of an external source $J(x)$. As an example, consider a quartically self interacting scalar field $\Phi$ on a periodic $D$-dimensional lattice, with Euclidean action

$$S_E(\Phi, J) = \sum_x \frac{1}{2} \sum_y \left( \Phi_x \left( -\Box + M^2 \right)_{x,y} \Phi_y \right) + \frac{g}{4} \Phi_x^4 - J_x \Phi_x ,$$

where

$$\left( -\Box + M^2 \right)_{x,y} \equiv (2D + M^2) \delta_{x,y} - \sum_{\hat{\mu}} \delta_{y,x+\hat{\mu}} .$$

The lattice spacing $a$ has been absorbed in the definition of the sources and parameters, and the $\hat{\mu}$ summation is over nearest neighbors. The generating function $Z(J)$ satisfies the following set of coupled partial differential equations in source space

$$\left( -\Box + M^2 \right)_{x,y} \frac{\partial Z}{\partial J_y} + g \frac{\partial^3 Z}{\partial J_x^3} - J_x Z = 0 .$$

There is one equation for each $J_x$. The Euclidean (unconnected) lattice Green’s functions can be extracted from $Z(J)$ by differentiation

$$\langle \Phi(x_1), \ldots, \Phi(x_m) \rangle = G_m(x_1, \ldots, x_m) = \frac{\partial^m Z}{\partial J_{x_1} \cdots \partial J_{x_m}} \bigg|_{J=0} \quad m = 1, 2, 3 \ldots .$$

For the rest of this note we will examine only $D = 1$ theories; the ideas generalize to higher dimensions. If fermions were present, the Grassman nature of the equations causes only technical complications.

3 Boundary Conditions

A straightforward way to attack \cite{3} is to construct a power series solution \cite{3}

$$Z(J_1, J_2, \ldots, J_N) = \sum_{n_1, n_2, \ldots, n_N} G_{n_1, n_2, \ldots, n_N} J_{1}^{n_1} J_{2}^{n_2} \cdots J_{N}^{n_N} ,$$

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with \( n_i, i = 1, 2, \ldots, N \) nonnegative integers.

Before solving (3) for the coefficients \( G_{n_1, n_2, \ldots, n_N} \), we must specify boundary conditions. Since (3) is homogeneous in \( Z \), we can normalize the vacuum amplitude

\[
Z(J = 0) = 1,
\]

and require odd Green's functions to vanish

\[
\langle \Phi_{x_1} \ldots \Phi_{x_n} \rangle = \left. \frac{\partial^n Z}{\partial J_{x_1} \ldots \partial J_{x_n}} \right|_{J = 0} = 0 \quad \forall J_x, n = 1, 3, 5 \ldots . \tag{7}
\]

If equation (3) is considered as an initial value problem, we need also to specify the second derivatives at the origin

\[
\langle \Phi_x \Phi_y \rangle = \left. \frac{\partial Z}{\partial J_x \partial J_y} \right|_{J = 0} . \tag{8}
\]

This appears to require a prior knowledge of the two point Green’s function [5].

Alternatively, we demand the constructed \( Z \) to approach smoothly the free field generating functional

\[
Z_0(J) = e^{J_x (-\triangle + M^2)^{-1} J_y} , \tag{9}
\]

when \( g \to 0^+ \). This requirement is an implicit boundary condition of all Monte-Carlo (path integral) simulations and, together with the above conditions, uniquely determines \( Z \). Other classes of solutions to the field equations ([5], [10], [7]) may also be of physical interest.

We found that one way of implementing this boundary condition is to truncate \( Z \) at some finite order \( K \) in the sources \( J \), so that all unconnected Green’s functions with more than \( K \) legs vanish. Truncation then introduces an approximation scheme which can be systematically improved by truncating at successively higher orders and taking the limit \( K \to \infty \). The convergence of this process will be discussed in future publications.

4 Lattice Symmetries

The number of coefficients in (3) grows exponentially with the number of sites and with increasing truncation order [8]. Consequently, this particular version of the Source Galerkin method is only of use for small lattices. We can get somewhat further by exploiting symmetries to reduce the number of unknowns to solve. For instance, in a lattice of ten sites, one can invoke translation and reflection
symmetries and group the 45 second order monomials of the form $J_x J_y$ into five invariant classes, thus reducing considerably the number of unknowns (see (19)).

Since the differential operators in (3) are closed under the action of the lattice symmetry group, it is natural to look only for invariant solutions $Z$.

$$Z(J) = \sum_\sigma \sum_n a_\sigma^{(n)}(J) P_\sigma^{(n)}(J),$$  \hspace{1cm} (10)

where $P_\sigma^{(n)}(J)$ are invariant polynomials of order $n$ corresponding to a particular symmetry class $\sigma$. The number of invariant classes for a given order will depend on both the number of lattice sites and on the number of symmetry operations for a given lattice. Details of how to construct these invariant polynomials will be given elsewhere, but it is important to realize now that they form a complete set for the class of lattice invariant solutions we are considering. We believe the ability to easily exploit symmetries is a major advantage of our approach.

Once $Z$ is constructed as lattice symmetric, it is sufficient to use only one equation from the coupled set (3): all equations in the coupled system express identical dynamics and only differ by lattice translations and reflections.

5 The Galerkin method

When solving a differential equation by power series methods, we substitute the series into the equation. Equating like terms in the resulting polynomial yields a system of linear algebraic equations that determine the expansion coefficients of the original power series.

Applying this procedure to (3) and the power series (10) for $Z$ yields an inconsistent set of linear equations for the truncated Green’s functions: there are more independent equations than unknowns $a_\sigma^{(n)}$. The Galerkin method is particularly suited to deal with this problem.

The key features of the Galerkin method can be stated concisely (11). Assume that we have a problem governed by a linear differential equation

$$L f = b.$$  \hspace{1cm} (11)

$L$ is a linear differential operator, and $b$ a known function of the $N$ variables $\mathbf{x} \equiv (x_1, \ldots, x_N)$. The solution is sought in a $N$-dimensional domain $\mathcal{D}$. The Galerkin method assumes that the exact solution $f = f(\mathbf{x})$ is accurately represented by an approximate $f_K^*$

$$f_K^*(\mathbf{a}; \mathbf{x}) = \varphi_0(\mathbf{x}) + \sum_{j=1}^K a_j \varphi_j(\mathbf{x}),$$  \hspace{1cm} (12)
where $\varphi_0$ is introduced to satisfy the boundary conditions and the $a_j$'s are coefficients to be determined. The $K$ functions $\varphi$ are selected according to some criterion, like knowledge of the approximate behavior of the solution or mathematical completeness. These are called basis, or trial, functions.

Substitution of (12) in (11) produces a nonzero residual $R$ given by

$$R(a; x) = L(f^*) = L(\varphi_0) + \sum_{j=1}^{K} a_j L(\varphi_j) .$$

(13)

The unknown coefficients $a_j$ are determined by solving the following system of linear algebraic equations

$$< \bar{\varphi}_k, R > = < \bar{\varphi}_k, b > ,$$

(14)

$$\sum_{j=1}^{K} < \bar{\varphi}_k, L \varphi_j > a_j = < \bar{\varphi}_k, b > - < \bar{\varphi}_k, L \varphi_0 > , \quad k = 1, 2, \ldots K ,$$

where $\bar{\varphi}$ are suitable test functions, and $< , >$ is the inner (scalar) product

$$< \phi, \chi > \equiv \int_{D} d^N x \phi \chi .$$

(15)

In the pure Galerkin method, the test functions are chosen from the same functional space as the basis functions $\varphi$ in (12).

Under very general conditions \[4\] it is possible to prove that the Galerkin solution $f_K^*$ converges to the true solution $f$ in the mean

$$\lim_{K \to \infty} \int_{D} ||f_K^* - f|| = 0 .$$

(16)

6 Example

As an illustration of the Galerkin method with truncated boundary conditions, we solve (3) for the case of a one dimensional lattice with three sites ($D = 1$ and $N = 3$ in (3)), expanding the generating function $Z$ up to the first non-trivial order in the sources, that is, up to quartic invariant polynomials.

First, we construct $Z_4^* = Z_4^*(J_1, J_2, J_3)$ as a linear combination of lattice invariant polynomials.

$$Z_4^*(J_1, J_2, J_3) = 1 + a_0^{(2)} P_0^{(2)}(J) + a_1^{(2)} P_1^{(2)}(J) + a_0^{(4)} P_0^{(4)}(J) + a_1^{(4)} P_1^{(4)}(J) + a_3^{(4)} P_3^{(4)}(J) ,$$

(17)

with

$$P_0^{(2)}(J) = J_1^2 + J_2^2 + J_3^2 ,$$

(18)
\[ P_4^{(2)}(J) = J_1 J_2 + J_2 J_3 + J_3 J_1, \]
\[ P_0^{(4)}(J) = J_1^4 + J_2^4 + J_3^4, \]
\[ \cdots. \]

Only six \( P_\sigma^{(n)} \) are needed. The boundary conditions in section 3 have already been imposed. We choose as our integration domain \( D = [-\epsilon, \epsilon]^3 \), a hypercube of size \( 2\epsilon \) centered at the origin, with \( \epsilon \) infinitesimal and set to zero after the calculation is done (this is of course possible only with algebraic languages like ALJABR, otherwise a numerical limit has to be taken).

Because the operator in (3) is odd and \( D \) is symmetric around \( J = 0 \), we need odd test functions in order to obtain non-vanishing inner products. A prescription for test functions that we found numerically convenient, since it provides the necessary number of independent equations for the coefficients \( a_\sigma^{(n)} \), is the derivative of the basis polynomials respect to a source \( J_x \)

\[ T_\sigma^{(n)} = \frac{\partial P_\sigma^{(n)}}{\partial J_x}. \tag{19} \]

Lattice symmetry makes any choice of \( x \) equivalent. We set \( x = 1 \). Any other set of test functions that produces the correct number of independent equations will also work, but with a different rate of convergence.

The Galerkin method is then applied to the residual of (3). The resulting coefficients \( a_\sigma^{(n)} \) are rational functions of the mass and the coupling. For instance, the Galerkin approximation to \( \langle \Phi(0)\Phi(0) \rangle \) is

\[ \langle \Phi(0)\Phi(0) \rangle^* = \frac{\partial Z^*_x}{\partial J_{J_1}} \bigg|_{J=0} = 2a_0^{(2)} \equiv \frac{A(M,g)}{B(M,g)}, \tag{20} \]

with

\[ A(M,g) = M^2(M^2 + 1)(M^2 + 3)(266M^4 + 929M^2 + 788) + 35g(M^2 + 1)(M^2 + 2)(14M^2 + 27), \tag{21} \]
\[ B(M,g) = M^4(M^2 + 3)^2(266M^4 + 929M^2 + 788) + g(1288M^8 + 7778M^6 + 17997M^4 + 18759M^2 + 7092) + 105g^2(M^2 + 1)(14M^2 + 27), \tag{22} \]

One can check that the above expression (20) has the right free field limit when \( g \to 0^+ \).
The convergence of this process is illustrated in Table 1, where we show our results for the two point function

\[ G_{i,j} = \langle \Phi_i \Phi_j \rangle = \frac{\partial^2 Z}{\partial J_i \partial J_j} \bigg|_{J=0}, \]

on an 11 site lattice with \( M = 1 \) and \( g = 0.5 \). We see that the results agree extraordinarily well with the Monte-Carlo simulation, and that the convergence is oscillatory \([7]\).

7 Conclusions

We have presented a new method to numerically attack problems in lattice QFT. It is not probabilistic and possesses extreme flexibility, allowing for maximum input of information (symmetry, spectral properties, etc.). Systematic improvements of the approximations are possible, forcing convergence (in the mean) to the exact solution. We have illustrated the method by looking at truncated Taylor series expansions. These lose tractability for big systems. We will present more useful nested approximations elsewhere.

The differential formulation requires treatment of boundary conditions. Truncation (among other boundary conditions \([7]\)) guarantees that the solution obtained from the differential equations corresponds to the solution of the path integral. Other types of solutions can also be analyzed with our method.

Finally, the Source Galerkin method gives real hope that lattice fermion theories will yield to numerical treatment. Monte Carlo approaches in QCD involving fermions are problematic. Calculation of the fermion determinant makes inclusion of dynamical quarks in lattice QCD prohibitive. Simulations of strongly correlated systems in condensed matter physics are afflicted by the minus sign problem \([9]\). We expect Source Galerkin to be a powerful tool for studying these systems since the above problems do not affect our method. The difference in computational complexity between bosons and fermions is minimal. Indeed, part of the strength of our method is the symmetry of approximations for bosons and fermions.

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[7] S. García and G. S. Guralnik, to be published; S. García, Brown University Ph.D. thesis.

[8] There are

$$\binom{N + d - 1}{d} = \frac{(N + d - 1)!}{(N - 1)! d!}$$

monomials of order $d$ in $N$ variables. Since the lattice symmetry group, the dihedral group, has $2N$ elements, one expects that the number of monomials not related by a lattice reflection or translation will be approximately

$$\frac{1}{2N} \binom{N + d - 1}{d} = \frac{(N + d - 1)!}{2 N! d!}.$$ 

The exact number, given by the cycle index of a polygon of $N$ sides, is close to this estimate. See N.G. De Bruijn, *Polya’s theory of Counting*, in Applied Combinatorial Mathematics (E.F. Beckenbach ed., John Wiley, New York, 1964); G.E. Andrews, The Theory of Partitions (Encyclopedia of Mathematics and its Applications, Volume 2, Addison-Wesley 1976).

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[11] See for instance chapter VII of C. Lanczos, Applied Analysis, (Dover, New York, 1988, reprint of the edition published by Prentice-Hall, 1956).
Table 1

| $i - j$ | $J^4$      | $J^6$      | $J^8$      | Shanks     | $M - C$         |
|---------|------------|------------|------------|------------|-----------------|
| 0       | 0.326538   | 0.360178   | 0.347223   | 0.35082    | $0.3510 \pm 0.0005$ |
| 1       | 0.094508   | 0.117673   | 0.108121   | 0.11091    | $0.1110 \pm 0.0004$ |
| 2       | 0.026768   | 0.038823   | 0.033422   | 0.03509    | $0.0351 \pm 0.0003$ |
| 3       | 0.007454   | 0.012940   | 0.010269   | 0.01114    | $0.0112 \pm 0.0004$ |
| 4       | 0.002075   | 0.004461   | 0.003197   | 0.00363    | $0.0036 \pm 0.0003$ |
| 5       | 0.000694   | 0.001922   | 0.001218   | 0.00147    | $0.0011 \pm 0.0004$ |

Table 1: Results for the two point function $G_{i,j}$ in a N=11 lattice (anharmonic oscillator). Columns: $|i - j|$, 4th., 6th. and 8th. order Galerkin approximations, numerical extrapolation (Shanks transformation) and Monte-Carlo data with statistical error.