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Solution of Operator Field Equations by the Method of Finite Elements

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A method is proposed for the approximate numerical solution of operator field equations on a lattice.

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Interest is rapidly growing in numerical quantum field theory. The emphasis has centered on evaluating functional integrals; one introduces a Euclidean space-time lattice to reduce the functional integral to an N-fold Riemann or Grassmann integral and performs a Monte Carlo evaluation of these integrals. A numerical evaluation of a functional integral is equivalent to solving an operator quantum field theory. However, this evaluation ignores operator properties of the theory such as the equal-time commutation relations (ETCR's). Rather, it is the summation over all possible classical configurations which elicits the characteristic properties of the quantum theory. Thus, an accurate evaluation of a functional integral requires a great many Monte Carlo passes through the lattice. In this paper, we present an alternative approach to the numerical solution of a quantum field theory, in which the operator field equations are solved directly on a Minkowski lattice. In our approach, we do operator time-stepping, which requires only one pass through the lattice.

We use the method of finite elements, a technique widely employed to solve numerically partial differential equations (PDE's) arising in classical continuum mechanics and fluid dynamics.[1] The method of finite elements consists of three steps: (i) Decompose the domain on which the PDE is to be solved into a set of contiguous nonoverlapping patches called finite elements. (ii) On each finite element approximate the solution to the PDE by a low-order polynomial. Adjust the coefficients of each polynomial so that the functions (and sometimes their derivatives) are continuous across adjacent patches. (iii) Impose the PDE at one point on every patch and impose boundary conditions on the patches adjacent to the boundary of the region. This procedure gives a system of algebraic equations for the coefficients of the polymonials. Solving these equations determines an approximate solution to the PDE.

The novelty of this paper is that we have been able to use this same technique to solve operator field equations. Now, the coefficients of the polynomials on the finite elements are operators, whose properties are determined by the ETCR's.

We illustrate the conventional finite-element procedure by solving a first-order differential equation: given $dy/dx = f(x, y)$ and $y(0) = y_0$, find $y(a)$ for $a > 0$. We introduce N finite elements of equal length $h = a/N$. On the kth finite element, where $x = (k-1)h + t$, $0 \leq t \leq h$, we represent the solution $y(x)$ by the linear function $y(x) = (1 - t/h)y_{k-1} + (t/h)y_k$. These functions form a continuous approximation to $y(x)$ for $0 \leq x \leq a$. Notice that on the first finite element, $y(x)$ satisfies the initial condition $y(0) = y_0$. We impose the differential equation at one point t_0, $0 \leq t_0 \leq h$, on each finite element. This gives the difference equation

$$(y_k - y_{k-1})/h = f((k-1)h + t_0, (1 - t_0/h)y_{k-1} + (t_0/h)y_k), \quad k = 1, \ldots, N. \tag{1}$$

To find $y(a) = y_N$, we repeatedly solve the algebraic equations (1) for the unknowns $y_1, y_2, y_3, \ldots, y_N$. As $N \to \infty$, y_N, the N-finite-element approximation to $y(a)$, becomes exact.

Now consider the problem of solving the Heisenberg equations of motion for a one-dimensional quantum system. If the Hamiltonian is

$$H = p^2/2 + V(q), \tag{2}$$

the Heisenberg equations are

$$dq(t)/dt = p(t), \quad dp(t)/dt = f(q(t)), \tag{3}$$

where $f(q) = -V'(q)$. The quantum mechanical problem consists of solving (3) for the operators $p(t)$ and $q(t)$ given the ETCR

$$[q(t), p(t)] = i. \tag{4}$$

We solve this problem first on a single finite element. We approximate $q(t)$ and $p(t)$ by linear functions of t:

$$\begin{aligned} q(t) &= (1 - t/h)q_0 + (t/h)q_1, \\ p(t) &= (1 - t/h)p_0 + (t/h)p_1, \\ 0 &\leq t \leq h. \end{aligned} \tag{5}$$

Substituting (5) into (3) and evaluating the result at the *center* of the time interval $t_0 = h/2$ gives

$$(q_1 - q_0)/h = \tfrac{1}{2}(p_0 + p_1), \tag{6}$$

$$(p_1 - p_0)/h = f(\tfrac{1}{2}(q_0 + q_1)). \tag{7}$$

Equations (6) and (7) are a discrete form of the equations of quantum mechanics. But, are they consistent with the ETCR's? At $t = 0$, (4) reads $[q_0, p_0] = i$. The question is, if we solve (6) and (7) simultaneously for the operators p_1 and q_1, will the commutator $[q_1, p_1]$ also have the value i? We can evaluate $[q_1, p_1]$ for any function f: Commute (6) on the right with $p_0 + p_1$,

$$[q_1 - q_0, p_0 + p_1] = 0, \tag{8}$$

and commute (7) on the left with $q_0 + q_1$,

$$[q_0 + q_1, p_1 - p_0] = 0. \tag{9}$$

Adding (8) and (9) gives

$$[q_1, p_1] = [q_0, p_0] = i. \tag{10}$$

Thus, we have proved that the method of finite elements *is* consistent with the ETCR's on a single finite element. Clearly, for a collection of N elements this argument may be iterated to show that the difference equations in (6) and (7) are consistent with the ETCR's in (4) at the end points of each of the finite elements.

We make two observations. First, the ETCR's hold only at the end points of a finite element, but not at any interior point. Second, the result in (10) depends crucially upon our having imposed the Heisenberg equations in (3) at the *center* of the finite element, $t = t_0 = h/2$. For any other value of t_0, (10) is false. Thus the operator properties of quantum mechanics uniquely determine the value of t_0. There is no such constraint on the value of t_0 for a c-number differential equation.[2]

Even though (6) and (7) are operator equations, we can solve them explicitly for p_1 and q_1, in terms of p_0 and q_0. First, we solve (6) for p_1:

$$p_1 = h^{-2}(q_1 - q_0) - p_0, \tag{11}$$

and use this result to eliminate p_1 from (7):

$$-\frac{2}{h}\,p_0 - \frac{4}{h^2}\,q_0 = g(\tfrac{1}{2}(q_1 + q_0)), \tag{12}$$

where $g(x) = f(x) - 4x/h^2$ is the function which completely characterizes the dynamical content of this quantum theory. The solution to (12) is given in terms of g^{-1}, where $g^{-1}(y)$ is the solution to the classical equation $y = g(x)$. From (12) we have

$$q_1 = -q_0 + 2g^{-1}(-(2/h)p_0 - (4/h^2)q_0) \tag{13}$$

and from (11) we obtain

$$p_1 = -p_0 - \frac{4}{h}\,q_0 + \frac{4}{h}\,g^{-1}(-(2/h)p_0 - (4/h^2)q_0). \tag{14}$$

The result in (13) and (14) is the one-time-step

solution of the quantum mechanical initial-value problem in (3).[3] We generalize to N time steps (N finite elements) by iterating (13) and (14) N times to express p_N and q_N in terms of p_0 and q_0. Note that the solution takes the form of a continued (nested) function $A+g^{-1}(A+g^{-1}(A+g^{-1}(A+\ldots)))$. If $[q_1, p_1]$ had not turned out to be i, but had differed from i by a (presumably) small q-number part that vanishes with the spacing h, then we would not be able to obtain the N-finite-element solution by iteration, and indeed we would not even be able to solve for p_2 and q_2.

Now we show how to generalize this method to quantum field theory. Consider a scalar field theory in two-dimensional Minkowski space. We write the operator field equations as a coupled first-order system so that we can continue to use linear approximations to the fields on finite elements:

$$\pi=\varphi_t,\quad \gamma=\varphi_x,\quad \pi_t-\gamma_x+f(\varphi)=0. \tag{15}$$

We introduce rectangular finite elements whose length in the time direction is h and in the space direction is k. On the m,n element, the field φ is approximated by the bilinear polynomial

$$\varphi(x,t)=\left(1+\frac{t}{h}\right)\left(1-\frac{x}{k}\right)\varphi_{m-1,n-1}+\left(1-\frac{t}{h}\right)\left(\frac{x}{k}\right)\varphi_{m,n-1}+\left(\frac{t}{h}\right)\left(1-\frac{x}{k}\right)\varphi_{m-1,n}+\left(\frac{t}{h}\right)\left(\frac{x}{k}\right)\varphi_{m,n}, \tag{16}$$

where the coefficient $\varphi_{m,n}$ is the value of the field operator at the site (m,n). The fields π and γ are represented in a similar way.

Our objective is to show how to advance one step in the time direction. We consider a single horizontal row of M finite elements and impose (15). The result is the following system of difference equations:

$$\begin{aligned}
&\tfrac{1}{4}(\pi_{m-1,0}+\pi_{m,0}+\pi_{m-1,1}+\pi_{m,1})=(2h)^{-1}(\varphi_{m,1}+\varphi_{m-1,1}-\varphi_{m,0}-\varphi_{m-1,0}),\\
&\tfrac{1}{4}(\gamma_{m-1,0}+\gamma_{m,0}+\gamma_{m-1,1}+\gamma_{m,1})=(2k)^{-1}(\varphi_{m,1}+\varphi_{m,0}-\varphi_{m-1,1}-\varphi_{m-1,0}),\\
&(2h)^{-1}(\pi_{m,1}+\pi_{m-1,1}-\pi_{m,0}-\pi_{m-1,0})-(2k)^{-1}(\gamma_{m,1}+\gamma_{m,0}-\gamma_{m-1,1}-\gamma_{m-1,0})\\
&\qquad=f\left(\tfrac{1}{4}(\varphi_{m-1,0}+\varphi_{m,0}+\varphi_{m-1,1}+\varphi_{m,1})\right),
\end{aligned} \tag{17}$$

$m=1,2,\ldots,M$. We take each finite element for φ and π to represent one degree of freedom and define the dynamical variables

$$\Phi_{m,n}=\tfrac{1}{2}(\varphi_{m,n}+\varphi_{m-1,n}),\quad \Pi_{m,n}=\tfrac{1}{2}(\pi_{m,n}+\pi_{m-1,n}). \tag{18}$$

If we eliminate $\gamma_{m,n}$ from (17) and express the resulting equations in terms of the dynamical variables we obtain a system of $2M$ equations whose general structure is

$$\Pi_{m,0}+\Pi_{m,1}=2h^{-1}(\Phi_{m,1}-\Phi_{m,0}), \tag{19}$$

$$\Pi_{m,1}-\Pi_{m,0}=\sum_{j=1}^{M}S_{m,j}(\Phi_{j,1}+\Phi_{j,0})+F(\Phi_{m,1}+\Phi_{m,0}), \tag{20}$$

$m=1,2,3,\ldots,M$. Here S is a symmetric matrix[4] and F is a nonlinear function simply related to f in (15).

When written in terms of $\Phi_{m,n}$ and $\Pi_{m,n}$, the ETCR's for the fields, $[\varphi(x,t),\pi(y,t)]=i\delta(x-y)$, become

$$\begin{aligned}
&[\Phi_{j,n},\Phi_{l,n}]=0,\quad [\Pi_{j,m},\Pi_{l,m}]=0,\\
&[\Phi_{j,m},\Pi_{l,m}]=(i/k)\delta_{j,l}.
\end{aligned} \tag{21}$$

The consistency problem here is to show that if (21) holds for $n=0$ then by virtue of (19) and (20) it also holds for $n=1$.

The proof of consistency is not simple. There are three steps. First, we eliminate $\Pi_{m,1}$, $m=1,2,3,\ldots,M$, from (20) using (19). Thus, (20) takes the form

$$\Pi_{m,0}+\frac{2}{h}\Phi_{m,0}=\sum_{j=1}^{M}S_{m,j}(\Phi_{j,1}+\Phi_{j,0})+G(\Phi_{m,1}+\Phi_{m,0}),\quad j=1,2,\ldots,M, \tag{22}$$

where G is simply related to F. Because

$$[\Pi_{j,0}+2h^{-1}\Phi_{j,0},\Pi_{l,0}+2h^{-1}\Phi_{l,0}]=0,$$

we can in principle solve (22) for $\Phi_{m,1}+\Phi_{m,0}$ in terms of $\Pi_{m,0}+2h^{-1}\Phi_{m,0}$. It follows from (21) at $n=0$ that

$$[\Phi_{j,1}+\Phi_{j,0},\Phi_{l,1}+\Phi_{l,0}]=0. \tag{23}$$

Second, we replace G in (22) by ϵG, where ϵ is a small parameter. Then, assuming that G has a Taylor series, we solve for $\Phi_{m,1}$ as a perturbation series in powers of ϵ. We can show that to all orders in powers of ϵ,

$$[\Phi_{j,1}, \Phi_{l,1}] = 0, \tag{24}$$

so long as S is a symmetric matrix. This is the difficult part of the proof.

Third, combining (23) and (24) gives

$$[\Phi_{j,1} - \Phi_{j,0}, \Phi_{l,1} - \Phi_{l,0}] = 0. \tag{25}$$

We complete the proof by using the same procedure as that leading to (10): We commute (19) and (20) with $\Phi_{j,0} \pm \Phi_{j,1}$ and add the resulting commutators to establish (21) for $n = 1$. It is quite interesting that this proof depends critically on the symmetry of the matrix S; the result is not sensitive to the choice of the nonlinear function f except for the assumption that it has a Taylor series expansion. Having established the consistency for the first time step, by induction (21) holds for all values of n. This proof also shows how to solve the operator equations (19) and (20) algebraically.

We conclude by illustrating the use of the finite-element approximation for some very simple systems, the harmonic oscillator, whose Hamiltonian is $H = p^2/2 + m^2q^2/2$, and the anharmonic oscillator, whose Hamiltonian is $H = p^2/2 + \lambda q^4/4$. For the harmonic oscillator, the operator equations (6) and (7) are linear and the solution in (13) and (14) can be written in matrix form: $(p_1, q_1) = M(p_0, q_0)$. M can be written as a similarity transform of a diagonal matrix D, $M = QDQ^{-1}$, whose entries are

$$d_{11}, d_{22} = (1 - \tfrac{1}{4}m^2h^2 \pm ihm)/(1 + \tfrac{1}{4}m^2h^2).$$

Thus the values of p and q after N time steps are determined by $M^N = QD^NQ^{-1}$; hence, q_N is a combination of $d_{11}{}^N$ and $d_{22}{}^N$. For $mh \ll 1$, we have $d_{11}{}^N$, $d_{22}{}^N = e^{\pm Nmhi}$. In the limit as $N \to \infty$ and $h \to 0$, $Nk = T$. Thus $q(T)$ is a linear combination of $e^{\pm imT}$, from which we can identify the energy gap $\Delta E = E_1 - E_0 = m$.

The energy gap for the anharmonic oscillator is known to be $\Delta E = E_1 - E_0 = (1.088\,45)\lambda^{1/3}$. We can calculate ΔE accurately from (6), (7), (10), and the equation

$$\langle n|p|m\rangle = i(E_n - E_m)\langle n|q|m\rangle,$$

where $|n\rangle$ is an eigenstate of the Hamiltonian H with energy E_n, using a variational procedure in which we increase the number of states and the number of time steps simultaneously. Using just one finite element we obtain $\Delta E = (\lambda/2)^{1/3} = (0.793\,70)\lambda^{1/3}$ which is 27% off. Two finite elements gives $\Delta E = (3\lambda/2)^{1/3} = (1.144\,71)\lambda^{1/3}$ which is 5% off.

More interesting than computing eigenvalues, we can apparently compute from the difference equations (17) unequal-time commutators, light-cone commutators, and S-matrix elements. We are working on these computations in various models.

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[1]G. Strang and G. J. Fix, *An Analysis of the Finite Element Method* (Prentice-Hall, Englewood Cliffs, N.J., 1973).

[2]Of course, requiring that Poisson brackets be preserved gives the same results for a classical Hamiltonian system.

[3]An intriguing question is whether (13) and (14) might be used in combination with $[q_0, p_0] = i$ to find a spectrum-generating algebra. Another interesting question is what to do when g^{-1} is multivalued.

[4]The matrix S is a numerical matrix containing the lattice spacings h and k. It is symmetric because with properly chosen boundary conditions the operator ∇^2 in the continuum is symmetric.