On the Discretization of Certain Operator Field Equations

Luis Vázquez

Departamento de Física Teórica, Facultad de Ciencias Físicas, Universidad Complutense, 28040 Madrid (Spain)

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Two new explicit finite difference schemes are proposed for certain operator field equations in a lattice.

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Recently Bender and Sharp [1, 2] presented 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. However the Bender-Sharp differencing scheme is implicit and computational difficulties arise. To avoid these problems Moncrief [3] has proposed a finite differencing scheme which is explicit preserving the canonical commutation relations. In this framework we propose two new methods of explicit finite differences which are related to that of Moncrief.

Let us start by considering a one-dimensional system

$$H = p^2/2 + V(q). (1)$$

The Heisenberg equations of motion are

$$dq(t)/dt = p(t), \quad dp(t)/dt = f(q(t)), \tag{2}$$

where f(q) = - dV/dq, and the operators p(t) and q(t) must satisfy the commutation relation

$$[q(t), p(t)] = i. (3)$$

In order to solve this problem in the interval [0, T] we divide it into N intervals of length τ . Now we will consider two explicit difference operator schemes which are consistent with (2)

Scheme I

$$\frac{q_{n+1} - q_n}{\tau} = p_n \,, \tag{4}$$

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$$\frac{p_{n+1} - p_n}{\tau} = f(q_{n+1}). \tag{5}$$

 q_n and p_n are the operators q and p at time $t = n \tau$.

Our problem is to iterate (4)-(5) with the initial condition

$$\{q_0, p_0\}$$
 such that $[q_0, p_0] = i$. (6)

From (4) with n = 0, and (6) we get the commutation relation

$$[q_0, q_1] = i \tau \tag{7}$$

that represents a discretization effect which also appears in the schemes of Bender-Sharp and Moncrief.

Now by commuting (5) with n = 0, on the left with q_1 and considering (7) we get

$$[q_1, p_1] = i. (8)$$

Iterating we obtain

$$[q_n, p_n] = i. (9)$$

Thus our scheme is explicit and preserves the equaltime commutation relations (ETCR) (3). On the other hand, no condition has to be imposed to the function f.

From (9) we obtain

$$[q_n, q_{n+1}] = i \tau.$$
 (10)

In this way we may reduce (4) and (5) to one equation which only contains the operators q_n :

$$\frac{q_{n+2} - 2q_{n+1} + q_n}{\tau^2} = f(q_{n+1}) \tag{11}$$

with the initial condition

$$\{q_0, q_1\}$$
 such that $[q_0, q_1] = i\tau$. (12)

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As it is well known, the local accuracy of a finite difference scheme is obtained by considering the difference between the exact solution of the differential and difference equations at the step n, with the help of Taylor's theorem. Applying that to (4) and (5) it is found that the scheme is accurate to order τ while if we consider (11) the scheme is accurate to order τ^2 . Thus the accuracy depends on the iteration being made either in terms of the operators $\{q_n, p_n\}$ or $\{q_n\}$ with the suitable commutation relations.

Finally we can approximate q(t) and p(t) in the interval $[n\tau, (n+1)\tau]$ as follows

$$q(t) = (n+1-t/\tau) q_n + (t/\tau - n) q_{n+1}, \quad (13)$$

$$p(t) = (n+1-t/\tau) p_n + (t/\tau - n) p_{n+1}.$$
 (14)

Scheme II

$$\frac{q_{n+1} - q_n}{\tau} = p_{n+1} \,, \tag{15}$$

$$\frac{p_{n+1} - p_n}{\tau} = f(q_n). {16}$$

Proceeding as in Scheme I we see that this scheme is explicit and preserves the ETCR with no conditions on the function f. On the other hand, if the iteration is made in terms of the operators $\{q_n\}$ with the commutation relation (10) we get the same second order operator equation (11). Thus the accuracy of schemes I and II is the same.

By comparing with Moncrief's scheme

$$\frac{q_{n+1} - q_n}{\tau} = p_n + \frac{1}{2} \tau f(q_n),$$
 (17)

$$\frac{p_{n+1} - p_n}{\tau} = \frac{1}{2} \left(f(q_n) + f(q_{n+1}) \right) \tag{18}$$

several remarks must be made.

- 1. If Moncrief's scheme were expressed in terms of the operators $\{q_n\}$ we would obtain the same second-order operator equation (11).
- 2. In terms of the operator $\{q_n, p_n\}$ Moncrief's scheme is accurate to order τ^2 while schemes I and II are accurate only to order τ . On the other hand, in terms of the operators $\{q_n\}$ the three schemes are accurate to order τ^2 .
- 3. Since the second order equation (11) is the same for the three schemes, the results about the

convergence of the solution obtained by Moncrief also hold for the schemes I and II.

Now we are going to apply our schemes in quantum field theory. For this purpose we consider a nonlinear scalar field theory in two-dimensional Minkowski space:

$$\Phi_t = \Pi, \quad \Pi_t - \Phi_{xx} - f(\Phi) = 0.$$
 (19)

In order to solve our field operator equations in a certain space-time region we discretize (19) by using a mesh of size $\Delta t = \tau$ and $\Delta x = h$ as follows:

Scheme I

$$\frac{\Phi_j^{n+1} - \Phi_j^n}{\tau} = \Pi_j^n, \tag{20}$$

$$\frac{\Pi^{n+1}}{\tau} = \frac{\Phi_{j+1}^{n+1} - 2\Phi_j^{n+1} + \Phi_{j-1}^{n+1}}{h^2} + f(\Phi_j^{n+1}), \tag{21}$$

where Φ_j^n and Π_j^n are the field operators at the point $(t = n\tau, x = jh)$.

The equal time commutation relations become

$$[\Phi_j^n, \Phi_k^n] = 0, \quad [\Pi_j^n, \Pi_k^n] = 0, \quad [\Phi_j^n, \Pi_k^n] = \frac{i}{h} \delta_{jk}.$$
 (22)

And we are going to show that if (19) holds for the step n, then it also holds for the step (n + 1).

From (20) and the relations (22) it is easy to get

$$[\Phi_i^{n+1}, \Phi_k^{n+1}] = 0. (23)$$

Now the discreteness effect is reflected in the commutation relation

$$[\boldsymbol{\Phi}_{j}^{n}, \boldsymbol{\Phi}_{k}^{n+1}] = i \frac{\tau}{h} \delta_{jk} \tag{24}$$

By commuting (21) on the left with Φ_k^{n+1} we obtain

$$[\Phi_k^{n+1}, \Pi_j^{n+1}] = \frac{i}{h} \, \delta_{kj} \,. \tag{25}$$

And from (20) we get

$$[\Pi_i^{n+1}, \Pi_k^{n+1}] = 0, (26)$$

which completes the proof of the consistence of our explicit scheme with the commutation relations.

Finally we define the fields in the rectangular finite elements determined by the lattice points (n, j), (n, j + 1), (n + 1, j) and (n + 1, j + 1) as

follows:

$$\Phi(t, x) = (n + 1 - t/\tau) (j + 1 - x/h) \Phi_{j}^{n}
+ (t/\tau - n) (x/h - j) \Phi_{j+1}^{n+1}
+ (x/h - j) (n + 1 - t/\tau) \Phi_{j+1}^{n}
+ (t/\tau - n) (j + 1 - x/h) \Phi_{j}^{n+1}.$$
(27)

The field Π is represented in a similar way. As we can see, the continuity of the fields across the adjacent patches is conserved.

Scheme II

The analogues of equations (15) and (16) are

$$\frac{\Phi_j^{n+1} - \Phi_j^n}{\tau} = \Pi_j^{n+1},\tag{28}$$

$$\frac{\Pi_j^{n+1} - \Pi_j^n}{\tau} = \frac{\Phi_{j+1}^n - 2\Phi_j^n + \Phi_{j-1}^n}{h^2} + f(\Phi_j^n). \tag{29}$$

[1] C. N. Bender and D. H. Sharp, Phys. Rev. Lett. 50, 1535 (1983).

[2] C. M. Bender, K. A. Milton, and D. H. Sharp, Phys. Rev. Lett. **51**, 1815 (1983).

[3] V. Moncrief, Phys. Rev. D 28, 2485 (1983).

Proceeding as before we see that the scheme also preserves the ETCR for a general function f. On the other hand both schemes may be reduced to an explicit second order finite difference scheme which only contains the operators Φ_i^n :

$$\frac{\Phi_{j}^{n+2} - 2\Phi_{j}^{n+1} + \Phi_{j}^{n}}{\tau^{2}}$$

$$= \frac{\Phi_{j+1}^{n+1} - 2\Phi_{j}^{n+1} + \Phi_{j-1}^{n+1}}{h^{2}} + f(\Phi_{j}^{n+1}) \quad (30)$$

with the initial condition

$$\{\boldsymbol{\Phi}_{j}^{0}, \boldsymbol{\Phi}_{j}^{1}\}, \text{ such that } [\boldsymbol{\Phi}_{k}^{0}, \boldsymbol{\Phi}_{j}^{1}] = i \frac{\tau}{h} \delta_{kj}.$$
 (31)

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