Journal of Statistical Physics, Vol. 60, Nos. 5/6, 1990

Explicit Runge–Kutta-like Schemes to Solve Certain Quantum Operator Equations of Motion

Qin Meng-Zhao and Zhang Mei-Qing

Received August 3, 1989; final March 20, 1990

We propose a kind of explicit sympletic Runge–Kutta-like scheme to solve operator equations of motion in quantum mechanics and in a quantum scalar field theory.

KEY WORDS: Heisenberg equations; symplectic method; Runge–Kutta method; ETCRs (equal-time commutation relations).

Interest is rapidly growing in numerical quantum field theory. Bender and Sharp[1,2] proposed a finite-difference approach to solving the operator equation of motion in quantum mechanics and in (lattice-regulated) quantum field theory. They show that, for a certain class of systems, their difference scheme, which is based on the finite-elements method of numerical approximation, exactly conserves the canonical equal-time commutation relations (ETCRs). However, the Bender–Sharp scheme is implicit and computational difficulties arise. Moncrief[3] and Vázquez[4] proposed some explicit schemes which are unitary and preserving the ETCRs.

The ETCRs are very important properties of the equation.

Bender *et al.*[8] applied the method to determine the spectrum for the underlying continuum theory. Applying an explicit scheme to the quantum field theory $\phi_{tt} - \phi_{xx} + (m^3/\sqrt{\lambda}) \sin[(\sqrt{\lambda}/m)\phi] = 0$ on a Minkowski lattice, Vázquez[9] obtained some estimates on the particle spectrum. Rogriguez and Vázquez[10] used the method to estimate the spectrum for the generalized quantum Hénon–Heiles system.

But all the schemes proposed are not of high order, and it would be

[1] Computing Center, Chinese Academy of Sciences, Beijing 100080 China.

0022-4715/90/0900-0839$06.00/0

of interest to find schemes that (1) are explicit, even for highly nonlinear systems, (2) preserve the ETCRs, even unitary, and (3) are of high order.

The purpose of this paper is to propose a kind of Runge–Kutta-like scheme which is explicit, of high order of accuracy, unitary, and preserves the ETCRs. Moreover, all the symplectic schemes in refs. 5–7 preserve the ETCRs.

Let us consider a one-dimensional quantum system

$$H = \tfrac{1}{2} p^2 + V(q) \tag{1}$$

The Heisenberg equations of motion are

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

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

$$[q(t), p(t)] = i \tag{3}$$

To solve this problem in the interval $[0, T]$, we divide it into N intervals of length τ and define q^n and p^n as the operators q and p at time $t = n\tau$.

Applying schemes which we obtained in ref. 7 to Eq. (2), we have the following Runge-Kutta-like schemes for Eq. (2).

One-stage method of order 1:

$$p^{k+1} = p^k + \tau c_1 f(q^k), \qquad q^{k+1} = q^k + \tau d_1 p^{k+1} \tag{s1}$$

where $c_1 = d_1 = 1$, $\tau = \Delta t$.

Two-stage method of order 2:

$$\begin{aligned} p_1 &= p^k + \tau c_1 f(q^k), & q_1 &= q^k + \tau d_1 p_1 \\ p^{k+1} &= p_1 + \tau c_2 f(q_1), & q^{k+1} &= q_1 + \tau d_2 p^{k+1} \end{aligned} \tag{s2}$$

where $c_1 = 0$, $c_2 = 1$, $d_1 = d_2 = \frac{1}{2}$, or $d_1 = 1$, $d_2 = 0$, $c_1 = c_2 = \frac{1}{2}$.

Three-stage method[11] of order 3:

$$\begin{aligned} p_1 &= p^k + \tau c_1 f(q^k), & q_1 &= q^k + \tau d_1 p_1 \\ p_2 &= p_1 + \tau c_2 f(q_1), & q_2 &= q_1 + \tau d_2 p_2 \\ p^{k+1} &= p_2 + \tau c_3 f(q_2), & q^{k+1} &= q_2 + \tau d_3 p^{k+1} \end{aligned} \tag{s3}$$

where

$$c_1 = \tfrac{7}{24}, \qquad c_2 = \tfrac{3}{4}, \qquad c_3 = -\tfrac{1}{24}$$

$$d_1 = \tfrac{2}{3}, \qquad d_2 = -\tfrac{2}{3}, \qquad d_3 = 1$$

or

$$c_1 = 1, \qquad c_2 = -\tfrac{2}{3}, \qquad c_3 = \tfrac{2}{3}$$
$$d_1 = -\tfrac{1}{24}, \qquad d_2 = \tfrac{3}{4}, \qquad d_3 = \tfrac{7}{24}$$

Four-stage method of fourth order of accuracy:

$$\begin{aligned} p_1 &= p^k + \tau c_1 f(q^k), & q_1 &= q^k + \tau d_1 p_1 \\ p_2 &= p_1 + \tau c_2 f(q_1), & q_2 &= q_1 + \tau d_2 p_2 \\ p_3 &= p_2 + \tau c_3 f(q_2), & q_3 &= q_2 + \tau d_3 p_3 \\ p^{k+1} &= p_3 + \tau c_4 f(q_3), & q^{k+1} &= q_3 + \tau d_4 p^{k+1} \end{aligned} \tag{s4}$$

$$c_1 = 0, \qquad c_2 = c_4 = \tfrac{1}{3}(2+\alpha), \qquad c_3 = -\tfrac{1}{3}(1+2\alpha)$$
$$d_1 = d_4 = \tfrac{1}{6}(2+\alpha), \qquad d_2 = d_3 = \tfrac{1}{6}(1-\alpha)$$

where $\alpha = 2^{1/3} + (1/2)^{1/3}$, or

$$c_1 = \tfrac{1}{6}(2+\alpha), \qquad c_2 = c_3 = \tfrac{1}{6}(1-\alpha), \qquad c_4 = \tfrac{1}{6}(2+\alpha)$$
$$d_1 = \tfrac{1}{3}(2+\alpha), \qquad d_2 = -\tfrac{1}{3}(1+2\alpha), \qquad d_3 = \tfrac{1}{3}(2+\alpha), \qquad d_4 = 0.$$

We note that scheme (s1) is a scheme which Vázquez[4] proposed.

ETCR and unitarity. First, let us consider the formal scheme

$$p_1 = p_0 + \tau c f(q_0), \qquad q_1 = q_0 + \tau d p_1 \tag{4}$$

where c and d are arbitrary constants, then

$$[q_1, p_1] = [q_0, p_1] = [q_0, p_0] \tag{5}$$

On the other hand,

$$q_1 = U^+ q_0 U, \qquad p_1 = U^+ p_0 U$$

where U is the unitary operator:

$$U = \exp\left[-\frac{c\tau}{h} V(q_0)\right] \exp\left(-\frac{d\tau}{2h} p_0^2\right)$$

This result follows from the results

$$\exp\left(\frac{d\tau}{2h} p_0^2\right) q_0 \exp\left(-\frac{d\tau}{2h} p_0^2\right) = q_0 + d\tau p_0$$

$$\exp\left[\frac{c\tau}{h} V(q_0)\right] p_0 \exp\left[-\frac{c\tau}{h} V(q_0)\right] = p_0 + c\tau f(q_0)$$

Now, we consider scheme (s4). The following relation can be easily found:

$$[q^{n+1}, p^{n+1}] = [q_3, p_3] = [q_2, p_2] = [q_1, p_1] = [q^n, p^n] \tag{6}$$

Our problem is to iterate the scheme with the initial condition

$$\{q_0, p_0\} \quad \text{such that} \quad [q_0, p_0] = i$$

From (6), we obtain

$$[q^n, p^n] = i \tag{7}$$

Thus, our schemes are explicit and unitary, and preserve the equal-time commutation relations (ETCRs). On the other hand, no condition has to be imposed on the function f.

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

$$q(t) = (n+1-t/\tau)\, q^n + (t/\tau - n)\, q^{n+1} \tag{8}$$

$$p(t) = (n+1-t/\tau)\, p^n + (t/\tau - n)\, p^{n+1} \tag{9}$$

Now we apply scheme (s4) to a nonlinear quantum scalar field theory in two-dimensional Minkowski space:

$$\Phi_t = \Pi, \qquad \Pi_t - \Phi_{xx} - f(\Phi) = 0 \tag{10}$$

In order to solve our field operator equations in a certain spacetime region, we discretize (10) by use a mesh of size $\Delta t = \tau$ and $\Delta x = h$ as follows:

$$\begin{aligned}
\Pi_j^{01} &= \Pi_j^n + \tau c_1 \left[\frac{\Phi_{j+1}^n - 2\Phi_j^n + \Phi_{j-1}^n}{h^2} + f(\Phi_j^n) \right] \\
\Phi_j^{01} &= \Phi_j^n + \tau d_1 \Pi_j^{01} \\
\Pi_j^{02} &= \Pi_j^{01} + \tau c_2 \left[\frac{\Phi_{j+1}^{01} - 2\Phi_j^{01} + \Phi_{j-1}^{01}}{h^2} + f(\Phi_j^{01}) \right] \\
\Phi_j^{02} &= \Phi_j^{01} + \tau d_2 \Pi_j^{02} \\
\Pi_j^{03} &= \Pi_j^{02} + \tau c_3 \left[\frac{\Phi_{j+1}^{02} - 2\Phi_j^{02} + \Phi_{j-1}^{02}}{h^2} + f(\Phi_j^{02}) \right] \\
\Phi_j^{03} &= \Phi_j^{02} + \tau d_3 \Pi_j^{03} \\
\Pi_j^{n+1} &= \Pi_j^{03} + \tau c_4 \left[\frac{\Phi_{j+1}^{03} - 2\Phi_j^{03} + \Phi_{j-1}^{03}}{h^2} + f(\Phi_j^{03}) \right] \\
\Phi_j^{n+1} &= \Phi_j^{03} + \tau d_4 \Pi_j^{n+1}
\end{aligned} \tag{11}$$

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

$$[\Phi_j^n, \Phi_k^n] = 0, \qquad [\Pi_j^n, \Pi_k^n] = 0, \qquad [\Phi_j^n, \Pi_k^n] = \frac{i}{h}\delta_{jk} \tag{12}$$

Since our scheme is symplectic, thus

$$\begin{aligned}
[\Phi_j^{n+1}, \Phi_k^{n+1}] &= [\Phi_j^n, \Phi_k^n] = 0 \\
[\Pi_j^{n+1}, \Pi_k^{n+1}] &= [\Pi_j^n, \Pi_k^n] = 0 \\
[\Phi_j^{n+1}, \Pi_k^{n+1}] &= [\Phi_j^n, \Pi_k^n] = \frac{i}{h}\delta_{jk}
\end{aligned} \tag{13}$$

Note that our scheme can be regarded as a combination of scheme (s1). It preserves the ECTRs.

Finally, we define the field 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:

$$\begin{aligned}
\Phi(t, x) = {} & (n+1-t/\tau)(j+1-x/h)\,\Phi_j^n \\
& + (t/\tau - n)(x/h - j)\,\Phi_{j+1}^{n+1} \\
& + (x/h - j)(n+1-t/\tau)\,\Phi_{j+1}^n \\
& + (t/\tau - n)(j+1-x/h)\,\Phi_j^{n+1}
\end{aligned}$$

The field Π is represented in a similar way, and the continuity of the fields across the adjacent patches is conserved.

Furthermore, one can obtain other schemes by the symplectic Runge–Kutta-like method.

ACKNOWLEDGMENT

This work was supported by the National Natural Science Foundation of China.

REFERENCES

1. C. M. 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. Mencrief, *Phys. Rev. D* **28**:2485 (1983).
4. L. Vázquez, *Z. Naturforsch.* **41a**:788 (1986).
5. Feng Kang, On difference scheme and symplectic geometry, in *Proceedings of the 1984 Beijing Symposium on Differential Geometry and Differential Equations—Computation of Partial Differential Equations*, Feng Kang, ed. (Science Press, Beijing, 1985), pp. 42–58.

6. Feng Kang and Qin Meng-zhao, The symplectic methods for the computation of Hamiltonian equations, in *Numerical Methods for Partial Differential Equations, Proc. Shanghai, 1986. Lecture Notes in Mathematics No. 1297*, Zhu You-lan and Gu Ben-yu, eds. (Springer, Berlin, 1987), pp. 1–37.
7. Qin Meng-zhao and Zhang Mei-qing, Sympectic Runge-Kutta schemes for Hamiltonian systems, to appear.
8. C. M. Bender, K. A. Milton, D. H. Sharp, L. M. Simmons, Jr., and R. S. Tong, *Phys. Rev. D* **32**:1476 (1985).
9. L. Vázquez, *Phys. Rev. D* **35**:35 (1987).
10. M. J. Rogriguez and L. Vázquez, Spectrum estimation for the generalized quantum Hénon–Heiles system, Second Howard University Symposium on Non-linear Semigroups, Partial Differential Equations and Attractors (August 1987).
11. R. D. Ruth, *IEEE Trans. on Nucl. Sci.* **NS-30**:2669–2671 (1983).