Computation of Quantum System by Second-Order Matrix Symplectic Scheme

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Received 18 December 2001; accepted 12 July 2001

DOI 10.1002/qua.10474

ABSTRACT: In this article the work of Vazquez and Zhang Meiqing et al. has been developed in such a way that it can be used to calculate time evolution of quantum system. In Heisenberg picture, operator symplectic schemes have been changed into matrix symplectic schemes by use of the expansion method, the matrix schemes satisfy equal time commutation relation (ETCR) in the matrix form. The second-order matrix scheme is used to calculate one-dimensional nonlinear harmonic oscillator. The calculated result is compared with results obtained by Runge–Kutta scheme. Calculated results show that results computed by ETCR-preserving and symplectic scheme is consistent with physics theory. It also shows that it is rational and effective as well as reliable to use ETCR-preserving symplectic scheme to calculate time evolution of quantum system in Heisenberg picture. It is proved that second-order symplectic scheme has more computing accuracy than does first-order symplectic scheme.

Key words: matrix; second order; symplectic scheme
Introduction

Symplectic algorithm to solve the classical Hamiltonian system is a difference algorithm that preserves the symplectic structure of the Hamiltonian system [1–6]. It has a particular advantage over nonsymplectic algorithm in long-time, multiple-step calculation. It has been successfully used in astronomy and plasma calculation [7, 8]. In Heisenberg picture, the coordinate operator \( q(t) \) and momentum operator \( p(t) \) of a quantum system satisfy

\[
\frac{d}{dt} q = \frac{1}{i\hbar} [q(t), H], \quad \frac{d}{dt} p = \frac{1}{i\hbar} [p(t), H]
\]

(1)

and the equal time commutation relation (ETCR)

\[
[q(t), p(t)] = i\hbar.
\]

(2)

In 1986, Vazquez [1] developed the work of Bender et al. [9, 10], as well as the work of Moncrief [11], for a quantum system

\[
H(p, q) = \frac{p^2}{2m} + V(q), \quad \frac{1}{i\hbar}[q(t), H] = \frac{p(t)}{m}
\]

\[
= H_q(p, q), \quad \frac{1}{i\hbar}[p(t), H] = -\nabla V(q) = -H_p(p, q),
\]

Heisenberg equations

\[
\frac{d}{dt} q = \frac{p}{m} = g(p), \quad \frac{d}{dt} p = -\nabla V(q) = -f(q)
\]

(3)

have the same form as classical canonical equations of Hamiltonian system. Vazquez proposed first-order explicit symplectic operator scheme of Eqs. (3)

\[
q^{n+1} = q^n + \frac{h}{m} p^n, \quad p^{n+1} = p^n - h\frac{\partial}{\partial q} V(q^n + hf(q^n))
\]

(4-1)

where \( h \) is step. It is proved that it must satisfy ETCR

\[
[q^n, p^n] = i\hbar
\]

(5)

Later, Mengzhao and Meiqing proposed second-order operator symplectic scheme [2, 3] of Eq. (3)

\[
y = p^n - \hbar c_2 f(q^n), \quad x = q^n + \hbar d_2 g(y)
\]

\[
p^{n+1} = y - \hbar c_2 f(x), \quad q^{n+1} = x + \hbar d_2 g(p^{n+1})
\]

(4-2)

where either \( c_1 = 0, c_2 = 1, d_1 = d_2 = 0.5, \) or \( c_1 = c_2 = 0.5, d_1 = 1.0, d_2 = 0.0. \) Because \( p(t) \) and \( q(t) \) are operators, they cannot be directly used in calculation. In 1999, Peizhu et al. [12] studied the matrix first-order symplectic scheme that satisfies ETCR. In this article, the work of Meiqing and Mengzhao has been developed such that the second-order operator scheme has been changed into second-order matrix scheme by expansion method, satisfying ETCR in matrix. This matrix scheme has been used in computing one-dimensional nonlinear harmonic oscillator

\[
H = \frac{p^2}{2m} + \frac{1}{2} \omega^2 q^2 + \frac{1}{4} A q^4.
\]

Let \( \omega = 1, m = 1, \) and \( h = 1, \) for simplicity. The computed result is compared with the result obtained by Runge–Kutta scheme. The computed results show that computed time evolution process of quantum system by ETCR-preserving and symplectic scheme is accurate and effective as well as strict. In Heisenberg picture, it preserves ETCR, although the computed total energy of the system is not conservative: it tends to ward accurate values as step \( h \) decreases. Both computed kinetic and potential energy are oscillating. In the process, when kinetic energy increases, potential energy decreases. When kinetic energy reaches it maximum value, potential energy reaches its minimum value. After that, kinetic energy decreases while potential energy increases. This computed result is consistent with theory and known results. But the total energy computed by Runge–Kutta method as time elapses is not consistent with energy conservation of the system.

Heisenberg Equations, ETCR, and Symplectic Scheme in Matrix Form

In Hilbert space for state of a quantum system, we choose complete basis of functions \( \Phi = \{ \phi_k \}_{k = 1, 2, \ldots} \), \( \{ \phi_k, \phi_k \} = \delta_{kk}. \) After \( q(t), p(t), \) and \( f(q(t)) \) are expanded in the functions of \( \Phi, \) we obtain

\[
q(t) \phi_j = \sum_k q_j(t) \phi_k, \quad p(t) \phi_j = \sum_k p_j(t) \phi_k, \quad f(q(t)) \phi_j = \sum_k f(q(t))_k \phi_k
\]

(6)
where \( q_{jk}(t) = (\phi_j, q(t)\phi_k), \) \( p_{jk}(t) = (\phi_j, p(t)\phi_k), \) \( f(q(t))_{jk} = (\phi_j, f(q(t))\phi_k). \) We substitute formula (6) into Heisenberg Eqs. (3) and ETCR (5). If we let \( N \) be great enough to do truncation, we obtain

\[
\frac{d}{dt} q_{jk}(t) = \frac{1}{m} p_{jk}(t) = g(p)_{jk}, \quad \frac{d}{dt} p_{jk}(t) = -f(q(t))_{jk},
\]

\( j, k = 1, 2, 3, \ldots, N \) \hspace{1cm} (7-1)

\[
\sum_{r=1}^{N} [q_{jr}(t)p_{rk}(t) - p_{jr}(t)q_{rk}(t)] = i\hbar \delta_{jk}, \quad j, k = 1, 2, 3, \ldots, N \hspace{1cm} (8-1)
\]

where \( f(q(t))_{jk} \) is matrix element. For example, if \( v(q) = (1/2)q^2 \), then \( v'(q) = f(q) = q \), we obtain matrix element \( f(q(t))_{jk} = q_{jk}(t) \). If \( v(q) = (1/2)q^2 + (1/4)Aq^4 \), then \( v'(q) = f(q) = q + Aq^3 \), we obtain matrix element \( f(q(t))_{jk} = q_{jk}(t) + A \sum_{r=1}^{N} q_{jr}(t)q_{rk}(t) \). Formulae (7-1) and (8-1) can be rewritten in matrix form

\[
\frac{d}{dt} [q_{jk}(t)] = \frac{1}{m} [p_{jk}(t)] = [g_{jk}(t)],
\]

\[
\frac{d}{dt} [p_{jk}(t)] = -[f(q(t))_{jk}], \hspace{1cm} (7-2)
\]

\[
[q_{jk}(t)], \quad [p_{jk}(t)] = i\hbar l, \hspace{1cm} (8-2)
\]

where \( I \) is \( N \times N \) unit matrix.

In form, formula (7-1) is Hamiltonian canonical equation, in time evolution process their solution keeps conservation of symplectic product. Symplectic schemes are difference schemes preserving symplectic product of Hamiltonian system, such as first-order explicit symplectic scheme [2, 6, 13, 14]

\[
p_{jk}^{n+1} = p_{jk}^n - \hbar f(q^n)_{jk}, \quad q_{jk}^{n+1} = q_{jk}^n + \hbar g(p^{n+1})_{jk}, \hspace{1cm} (9-1)
\]

and second-order symplectic scheme

\[
y_{jk}^{n} = y_{jk}^n - \hbar c_1 f(q^n)_{jk}, \quad x_{jk}^{n} = x_{jk}^n + \hbar d_{1}g(y^n)_{jk},
\]

\[
p_{jk}^{n+1} = y_{jk}^{n} - \hbar c_2 f(x^n)_{jk}, \quad q_{jk}^{n+1} = x_{jk}^{n} + \hbar d_{2}g(p^{n+1})_{jk}, \hspace{1cm} (9-2)
\]

where either \( c_1 = 0, c_2 = 1, d_1 = d_2 = 0.5 \) or \( c_1 = c_2 = 0.5, d_1 = 1.0, d_2 = 0.0 \). It can be proved by mathematical induction that second-order explicit scheme (9-2) satisfies matrix ETCR (8)

\[
\sum_{r=1}^{N} [q_{jr}^n p_{rk}^n - p_{jr}^n q_{rk}^n] = i\hbar \delta_{jk}, \hspace{1cm} (10)
\]

In the same way, the second-order explicit symplectic scheme

\[
x_{jk}^{n} = x_{jk}^n + \hbar c_1 g(p^n)_{jk}, \quad y_{jk}^{n} = y_{jk}^n + \hbar d_{1}f(x^n)_{jk},
\]

\[
p_{jk}^{n+1} = y_{jk}^{n} + \hbar c_2 g(y^n)_{jk}, \quad q_{jk}^{n+1} = x_{jk}^{n} + \hbar d_{2}f(p^{n+1})_{jk}, \hspace{1cm} (11)
\]

where either \( c_1 = 0, c_2 = 1, d_1 = d_2 = 0.5 \), or \( c_1 = c_2 = 0.5, d_1 = 1.0, d_2 = 0.0 \) also satisfies ETCR (10).

So the scheme (9-2) and scheme (11) are second-order matrix ETCR-preserving and symplectic scheme.

### Computation and Discussion of One-Dimensional Nonlinear Harmonic Oscillator by Second-Order Matrix ETCR-Preserving and Symplectic Scheme

We start considering one-dimensional nonlinear oscillator

\[
H = \frac{p^2}{2} + \frac{q^2}{2} + \frac{1}{4} A q^4 \hspace{1cm} (12)
\]

where \( A = 0.01 \). Its Heisenberg equations can be written as follows

\[
\frac{d}{dt} q = p, \quad \frac{d}{dt} p = -f(q), \quad f(q) = q + A q^3 \hspace{1cm} (13)
\]

We choose eigenvalue problem of one-dimensional harmonic oscillator

\[
H_0 = \frac{p^2}{2} + \frac{q^2}{2}, H_0 y_n = E_n y_n, \quad E_n = n + \frac{1}{2},
\]

\[
y_n = \pi^{-1/4} (2n)!^{1/2} \left[ \exp \left(-\frac{q^2}{2}\right) \right] h_n(x) n = 0, 1, 2, \ldots
\]

where \( h_n(x) \) is Hermite polynomial. The set of eigenfunctions \( Y = \{y_n, n = 0, 1, 2, \ldots \} \) is orthonor-
mal complete basis, \( q(t) \) and \( p(t) \) are expanded in the basis \( Y \). If we let \( N \) be great enough to do truncation, we obtain Heisenberg equations in matrix element form

\[
\frac{d}{dt} q_{jk} = p_{jr} \quad \frac{d}{dt} p_{jk} = -f(q)_{jk}
\]  

(14)

where \( f(q)_{jk} = q_{jk} + A \sum_{r,s=1}^{N} q_{jr} q_{rs} q_{skr} \) we also obtain ETCR in matrix form

\[
\sum_{r=1}^{N} [q_{jr}(t)p_{rk}(t) - p_{jr}(t)q_{rk}(t)] = i\delta_{jk}
\]  

(15)

We expand initial coordinate operator \( q(0) = q_0 \) and initial momentum operator \( p(0) = p_0 \) by Hermite polynomial recursion relation, we obtain following initial conditions

\[
N=10, \ h=0.01 \ T
\]

FIGURE 1. Second-order Runge–Kutta scheme (\( n = 10; \ h = 0.01 \ T \)).

FIGURE 2. Second-order symplectic scheme (\( c_1 = 0.5, c_2 = 0.5, d_1 = 1, d_2 = 0 \)).

FIGURE 3. Second symplectic scheme (\( c_1 = 0.5, c_2 = 0.5, d_1 = 1, d_2 = 0 \)).

FIGURE 4. Second-order symplectic scheme (\( c_1 = 0.5, c_2 = 0.5, d_1 = 0.5, d_2 = 0 \)).
A state $\tilde{\Psi} = a_0 \psi_0 + a_1 \psi_1 + a_2 \psi_2$ is chosen as initial state of nonlinear oscillator where $a_0 = 0.5345225$, $a_1 = 0.8017837$, $a_2 = 0.2672612$. $T = 2\pi$ is period of corresponding linear oscillator $H_0$. Let step $h = T \times 10^{-2}, T \times 10^{-3}, T \times 10^{-4}$ in turn. Let $N = 11, 21$ in turn to do truncation. By means of second-order ETCR-preserving and symplectic scheme (9-2) and Runge–Kutta scheme, both matrix elements of coordinate operator and matrix elements of momentum operator have been computed, ETCR has checked by formula

$$c_{jk}^{n} = \sum_{r=1}^{N} [q_{jr}^{n} p_{rk}^{n} - p_{jr}^{n} q_{rk}^{n}] = i \delta_{jk}. $$

Meanwhile, time evolution of kinetic energy

$$T^{n} = \sum_{j=1}^{N} \sum_{k=1}^{N} \left( \frac{1}{2} \sum_{r=1}^{N} [p_{jr}^{n} p_{rk}^{n}] \right),$$

time evolution of potential energy

$$V^{n} = \sum_{j=1}^{N} \sum_{k=1}^{N} \left( \frac{1}{2} \sum_{r=1}^{N} [q_{jr}^{n} q_{rk}^{n}] \right) + \frac{1}{4} \sum_{r=1}^{N} \sum_{s=1}^{N} \sum_{t=1}^{N} [q_{jr}^{n} q_{rs}^{n} q_{st}^{n} q_{tk}^{n}],$$

and time evolution of total energy

$$H^{n} = T^{n} + V^{n}$$

have been computed, respectively.

Figures 1–5 show the computed results. Figure 1 shows that total energy and kinetic energy as well as potential energy by Runge–Kutta scheme increases with time, which is not consistent with the fact that the energy is conservative. Figure 2 shows that although the symplectic scheme (9-2) cannot preserve total energy strictly, computed total energy oscillates about average value greater than exact value, when $c_1 = 0, c_2 = 1, d_1 = 0.5, d_2 = 0.5$. Computed total energy oscillates about an average value less than exact value, if $c_1 = 0.5, c_2 = 0.5, d_1 = 1, d_2 = 0$, as shown in Figure 3. Oscillation amplitude and max $|H^n - H^0|$ tend to zero as step $h$ decreases. Therefore, for a given accuracy, provided that step $h$ is properly reduced, ETCR-preserving and symplectic scheme keeps total energy conservative. Figure 4 shows that potential energy and kinetic energy oscillate periodically. When kinetic energy increases, potential energy decreases. When kinetic energy reaches its maximum value, potential energy reaches its minimum value, then kinetic energy decreases while potential energy increases. The result is consistent with theory. The computed results also show that ETCR-preserving and symplectic scheme (9-2) satisfies ETCR (8-1), but Runge–Kutta method made the imaginary part of every diagonal matrix element $c_{jk}^{n}$ become greater as time elapses. Second-order scheme greatly improved accuracy of computation in comparison with first symplectic scheme, as shown in Figure 5.

**Conclusion**

The work of L. Vazquez and the work of Zhang Weiqing have been developed in this article. In Heisenberg picture, second-order operator symplectic scheme has been changed into second-order matrix symplectic scheme. The scheme satisfies ETCR in matrix form. Second-order matrix sym-
plectic scheme is more accurate than first-order matrix symplectic scheme. Therefore, their work was developed for use in computing quantum system time evolution. It is shown in this work that an interaction picture preserving structure algorithm can be set up, provided that the ETCR-preserving and symplectic scheme in Heisenberg picture is combined with the symplectic and square-preserving scheme in Schrödinger picture.

ACKNOWLEDGEMENTS

This work was supported by both National Natural Science Foundation of China (codes: 10074019 and 10171039) and The Special Funds for Major State Basic Research Projects (code: G1999032804).

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