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Explicit Unitary Schemes to Solve Quantum Operator Equations of Motion

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To solve operator equations of motion in quantum mechanics and in a quantum scalar field theory, we propose an explicit unitary scheme with arbitrary high order of accuracy.

KEY WORDS: Heisenberg equations; unitarity; explicit unitary scheme; ETCRs (equal-time commutation relations).

Bender and Sharp[1,2] proposed a finite-difference approach to solve operator equations 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, therefore Moncrief,[3] Vázquez,[4] and Qin and Zhang[14] proposed explicit schemes which are unitary and preserve the ETCRs.

ETCRs are very important properties of the equation.

Bender *et al.*[10] 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[11] obtained some estimates on the particle spectrum. Rogriguez and Vázques[12] used the method to estimate the spectrum for the generalized quantum Hénon–Heiles system.

But not all the explicit schemes proposed are of high order, and only for systems with energy $H = \frac{1}{2}P^2 + V(q)$ or $H = H_0(p, q) + V(q)$, where H_0 is a solvable system, and it would be of interest to find schemes that (1) are

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explicit, even for highly nonlinear systems, (2) preserve unitary, and thus the ETCRs, (3) are of high order, and (4) are applicable to a wide class of systems.

Here we propose an explicit unitary scheme, in which all proposed explicit unitary schemes can be expressed.

Let us consider a one-dimensional quantum system

$$H = H_1(p, q) + H_2(p, q) \tag{1}$$

where H_1 and H_2 are solvable systems. The Heisenberg equations of system (1) are

$$\begin{aligned} \frac{dq(t)}{dt} &= \frac{1}{ih}[q, H_1 + H_2] = \frac{1}{ih}[q, H_1] + \frac{1}{ih}[q, H_2] \\ \frac{dp(t)}{dt} &= \frac{1}{ih}[p, H_1 + H_2] = \frac{1}{ih}[p, H_1] + \frac{1}{ih}[p, H_2] \end{aligned} \tag{2}$$

We consider systems H_1 and H_2 separately. The Heisenberg equations of system H_1 are

$$\frac{dq(t)}{dt} = \frac{1}{ih}[q, H_1], \qquad \frac{dp(t)}{dt} = \frac{1}{ih}[p, H_1] \tag{3}$$

H_1 is solvable, i.e., system (3) has an exact soluation

$$\begin{aligned} q(t) &= f_1(q_0, p_0, t) = \exp\left(\frac{it}{h} H_1\right) q_0 \exp\left(-\frac{it}{h} H_1\right) \\ p(t) &= g_1(q_0, p_0, t) = \exp\left(\frac{it}{h} H_1\right) p_0 \exp\left(-\frac{it}{h} H_1\right) \end{aligned} \tag{4}$$

The Heisenberg equations of system H_2 are

$$\frac{dq(t)}{dt} = \frac{1}{ih}[q, H_2], \qquad \frac{dp(t)}{dt} = \frac{1}{ih}[p, H_2] \tag{5}$$

System (5) has an exact soluation

$$\begin{aligned} q(t) &= f_2(q_0, p_0, t) = \exp\left(\frac{it}{h} H_2\right) q_0 \exp\left(-\frac{it}{h} H_2\right) \\ p(t) &= g_2(q_0, p_0, t) = \exp\left(\frac{it}{h} H_2\right) p_0 \exp\left(-\frac{it}{h} H_2\right) \end{aligned} \tag{6}$$

To solve system (1) in the interval $[0, T]$, we divide it into N intervals of length τ and define q^k and p^k as the operators q and p at time $t = k\tau$.

We construct the following explicit unitary schemes:

1. *Schemes of first order of accuracy*: $ZM_{1\text{st}}(\tau)$ and $ZQ_{1\text{st}}(\tau)$.

One scheme is

$$\begin{aligned} q_1 &= f_1(q^k, p^k, \tau), & p_1 &= g_1(q^k, p^k, \tau) \\ q^{k+1} &= f_2(q_1, p_1, \tau), & p^{k+1} &= g_2(q_1, p_1, \tau) \end{aligned} \tag{7}$$

and we denote scheme (7) $ZM_{1\text{st}}(\tau)$. This scheme can be expressed in the following form:

$$q^{k+1} = U_1^+(\tau)\, q^k U_1(\tau), \qquad p^{k+1} = U_1^+(\tau)\, p^k U_1(\tau) \tag{7'}$$

where

$$U_1(\tau) = \exp\left(-\frac{i\tau}{h} H_1\right) \exp\left(-\frac{i\tau}{h} H_2\right)$$

Thus the scheme is unitary and satisfies the ETCRs.

From the Baker–Campbell–Hausdorff (BCH) formula[15]

$$\begin{aligned} &\exp\left(-\frac{i\tau}{h} H_1\right) \exp\left(-\frac{i\tau}{h} H_2\right) \\ &\quad = \exp\left\{-\frac{i\tau}{h}(H_1 + H_2) + \frac{1}{2}\left(-\frac{i\tau}{h}\right)^2 [H_1, H_2] + \cdots\right\} \\ &\quad = \exp\left[-\frac{i\tau}{h}(H_1 + H_2)\right] + o(\tau^2) \end{aligned}$$

Therefore, the local error of scheme (7) with respect to time τ is $o(\tau^2)$, i.e., scheme (7) is of order 1. Another scheme of order 1 is

$$\begin{aligned} q_1 &= f_2(q^k, p^k, \tau), & p_1 &= g_2(q^k, p^k, \tau) \\ q^{k+1} &= f_1(q_1, p_1, \tau), & p^{k+1} &= g_1(q_1, p_1, \tau) \end{aligned} \tag{8}$$

we denote scheme (8) $ZQ_{1\text{st}}(\tau)$.

2. *Schemes of second order of accuracy*: $ZM_{2\text{nd}}(\tau)$ and $ZQ_{2\text{nd}}(\tau)$.

If we have two schemes $A(\tau)$ and $B(\tau)$ for system (1), we can compound a scheme $B(\tau_2)\, A(\tau_1)$ of $A(\tau)$ and $B(\tau)$, i.e., first we implement scheme $A(\tau)$ with initial q^k, p^k, and step τ_1, and get results q_1, p_1. Then we implement scheme $B(\tau)$ with initial q_1, p_1, and step τ_2 and get the final result q^{k+1}, p^{k+1}.

We use the composition of $ZM_{1st}(\tau)$ and $ZQ_{1st}(\tau)$ to construct a scheme of second order. The scheme is $ZM_{2nd}(\tau) = ZQ_{1st}(c_{11}\tau)\, ZM_{1st}(c_{12}\tau)$, where $c_{11} = c_{12} = 1/2$, i.e.,

$$\begin{aligned} q_1 &= f_1(q^k, p^k, \tau/2), & p_1 &= g_1(q^k, p^k, \tau/2) \\ q_2 &= f_2(q_1, p_1, \tau/2), & p_2 &= g_2(q_1, p_1, \tau/2) \\ q_3 &= f_2(q_2, p_2, \tau/2), & p_3 &= g_2(q_2, p_2, \tau/2) \\ q^{k+1} &= f_1(q_3, p_3, \tau/2), & p^{k+1} &= g_1(q_3, p_3, \tau/2) \end{aligned} \tag{9}$$

or

$$\begin{aligned} q_1 &= f_1(q^k, p^k, \tau/2), & p_1 &= g_1(q^k, p^k, \tau/2) \\ q_2 &= f_2(q_1, p_1, \tau), & p_2 &= g_2(q_1, p_1, \tau) \\ q^{k+1} &= f_1(q_2, p_2, \tau/2), & p^{k+1} &= g_1(q_2, p_2, \tau/2) \end{aligned} \tag{10}$$

This scheme can be expressed in the following form:

$$q^{k+1} = U_2^{+}(\tau)\, q^k U_2(\tau), \qquad p^{k+1} = U_2^{+}(\tau)\, p^k U_2(\tau) \tag{10'}$$

where

$$U_2(\tau) = \exp\left(-\frac{i\tau}{2h} H_1\right) \exp\left(-\frac{i\tau}{h} H_2\right) \exp\left(-\frac{i\tau}{2h} H_1\right)$$

By BCH formula, one can easily obtain that

$$U_2(\tau) = \exp\left[-\frac{i\tau}{h}(H_1 + H_2)\right] + o(\tau^3)$$

i.e., scheme (10) is a scheme of order 2. Moreover, $U_2(-\tau)\, U_2(\tau) = I$, which means that scheme (10) is time-reversible.

Using the composition of $ZQ_{1st}(\tau)$ and $ZM_{1st}(\tau)$, we construct another scheme of second order. The scheme is $ZQ_{2nd}(\tau) = ZM_{1st}(c_{11}\tau)\, ZQ_{1st}(c_{12}\tau)$, where $c_{11} = c_{12} = 1/2$, i.e.,

$$\begin{aligned} q_1 &= f_2(q^k, p^k, \tau/2), & p_2 &= g_2(q^k, p^k, \tau/2) \\ q_2 &= f_1(q_1, p_1, \tau), & p_2 &= g_1(q_1, p_1, \tau) \\ q^{k+1} &= f_2(q_2, p_2, \tau/2), & p^{k+1} &= g_2(q_2, p_2, \tau/2) \end{aligned} \tag{11}$$

3. *Schemes of fourth order of accuracy*: $ZM_{4th}(\tau)$ and $ZQ_{4th}(\tau)$.

Using the composition of $ZM_{2nd}(\tau)$ with step $c_{21}\tau$, $c_{22}\tau$, $c_{21}\tau$, respectively, we construct a scheme of 4th order of accuracy

$$ZM_{4th}(\tau) = ZM_{2nd}(c_{21}\tau)\, ZM_{2nd}(c_{22}\tau)\, ZM_{2nd}(c_{21}\tau) \tag{12}$$

From the BCH formula, expecting scheme (12) to be of 4th order of accuracy, we take $c_{21}=1/(2-2^{1/3})$, $c_{22}=-2^{1/3}(2-2^{1/3})$.

Using the composition of $ZQ_{2\text{nd}}(\tau)$ with steps $c_{21}\tau$, $c_{22}\tau$, $c_{21}\tau$, respectively, we construct another scheme of 4th order

$$ZQ_{4\text{th}}(\tau)=ZQ_{2\text{nd}}(c_{21}\tau)\,ZQ_{2\text{nd}}(c_{22}\tau)\,ZQ_{2\text{nd}}(c_{21}\tau) \tag{13}$$

4. *Schemes of sixth order of accuracy*: $ZM_{6\text{th}}(\tau)$ and $ZQ_{6\text{th}}(\tau)$:

$$ZM_{6\text{th}}(\tau)=ZM_{4\text{th}}(c_{31}\tau)\,ZM_{4\text{th}}(c_{32}\tau)\,ZM_{4\text{th}}(c_{31}\tau) \tag{14}$$

$$ZQ_{6\text{th}}(\tau)=ZQ_{4\text{th}}(c_{31}\tau)\,ZQ_{4\text{th}}(c_{32}\tau)\,ZQ_{4\text{th}}(c_{31}\tau) \tag{15}$$

where $c_{31}=1/(2-2^{1/5})$, $c_{32}=-2^{1/5}/(2-2^{1/5})$.

5. *Schemes of 2nth order of accuracy*: $ZM_{2n\text{th}}(\tau)$ and $ZQ_{2n\text{th}}(\tau)$.

More generally, if a scheme of order $2(n-1)$ is already known, we can obtain a scheme of order $2n$ by the composition.

$$ZM_{2n\text{th}}(\tau)=ZM_{2(n-1)\text{th}}(c_{n1}\tau)\,ZM_{2(n-1)\text{th}}(c_{n2}\tau)\,ZM_{2(n-1)\text{th}}(c_{n1}\tau) \tag{16}$$

$$ZQ_{2n\text{th}}(\tau)=ZQ_{2(n-1)\text{th}}(c_{n1}\tau)\,ZQ_{2(n-1)\text{th}}(c_{n2}\tau)\,ZM_{2(n-1)\text{th}}(c_{n1}\tau) \tag{17}$$

where $c_{n1}=1/(2-2^{1/(2n-1)})$ and $c_{n2}=-2^{1/(2n-1)}/(2-2^{1/(2n-1)})$. We thank H. Yoshida[9] for calculating these coefficients for a special type of classical Hamiltonian system. Qin and Zhu[16] show that these coefficients are valid for general classical Hamiltonian systems and some general schemes; we can show that these coefficients are also valid for our proposed schemes and Hamiltonian systems. The proofs will be given in another paper, and are pure mathematical calculations of commutators.

Remarks. (1) If $H=H_1+H_2+\cdots+H_n$, the Heisenberg equation of motion for the system H_i has an exact solution

$$\begin{aligned} q(t)&=f_i(q_0,p_0,t)=\exp\left(\frac{it}{h}H_i\right)q_0\exp\left(-\frac{it}{h}H_i\right)\\ p(t)&=g_i(q_0,p_0,t)=\exp\left(\frac{it}{h}H_i\right)p_0\exp\left(-\frac{it}{h}H_i\right)\end{aligned} \tag{18}$$

Let $[s_1, s_2,..., s_n]$ be an arbitrary permutation of $[1, 2,..., n]$; we construct $ZM_{1\text{st}}$ and $ZQ_{1\text{st}}$, respectively, in the following forms:

$ZM_{1\text{st}}(\tau)$:

$$\begin{aligned} q_1&=f_{s_1}(q^k,p^k,\tau), & p_1&=g_{s_1}(q^k,p^k,\tau)\\ q_2&=f_{s_2}(q_1,p_1,\tau), & p_2&=g_{s_2}(q_1,p_1,\tau)\\ &\cdots & &\cdots\\ q^{k+1}&=f_{s_n}(q_{n-1},p_{n-1},\tau), & p^{k+1}&=g_{s_n}(q_{n-1},p_{n-1},\tau)\end{aligned} \tag{19}$$

$ZQ_{1st}(\tau)$:

$$\begin{aligned} q_1 &= f_{s_n}(q^k, p^k, \tau), & p_1 &= g_{s_n}(q^k, p^k, \tau) \\ q_2 &= f_{s_{n-1}}(q_1, p_1, \tau), & p_2 &= g_{s_{n-1}}(q_1, p_1, \tau) \\ &\cdots & &\cdots \\ q^{k+1} &= f_{s_1}(q_{n-1}, p_{n-1}, \tau), & p^{k+1} &= g_{s_1}(q_{n-1}, p_{n-1}, \tau) \end{aligned} \tag{20}$$

These schemes are explicit and unitary. Following the above approach, we can construct high-order schemes for $H = H_1 + H_2 + \cdots + H_n$ by the compositions of $ZQ_{1st}(\tau)$ and $ZM_{1st}(\tau)$.

(2) Applying these schemes to a nonlinear quantum scalar field theory in two-dimensional Minkowski space

$$\Phi_t = \Pi, \qquad \Pi_t - \Phi_{xx} - f(\Phi) = 0 \tag{21}$$

we can obtain a series of explicit unitary schemes for (21); for example, we break up the Hamiltonian

$$H = \int dx(1/2\Phi_x^2 + 1/2\Pi^2 + V(\Phi))$$

into $H_1 = \int dx(1/2\Phi_x^2 + V(\Phi))$ and $H_2 = \int dx\, \Pi^2/2$. The ZM_{1st} and ZQ_{1st} are constructed, respectively, in the following forms:

$ZM_{1st}(\tau)$:

$$\begin{aligned} \Pi_j^{01} &= \Pi_j^n + \tau\left[\frac{\Phi_{j+1}^n - 2\Phi_j^n + \Phi_{j-1}^n}{h^2} + f(\Phi_j^n)\right] \\ \Phi_j^{01} &= \Phi_j^n \\ \Phi_j^{n+1} &= \Phi_j^{01} + \tau\Pi_j^{01} \\ \Pi_j^{n+1} &= \Pi_j^{01} \end{aligned} \tag{22}$$

i.e.,

$$\begin{aligned} \Pi_j^{n+1} &= \Pi_j^n + \tau\left[\frac{\Phi_{j+1}^n - 2\Phi_j^n + \Phi_{j-1}^n}{h^2} + f(\Phi_j^n)\right] \\ \Phi_j^{n+1} &= \Phi_j^n + \tau\Pi_j^{n+1} \end{aligned} \tag{23}$$

$ZQ_{1st}(\tau)$:

$$\begin{aligned} \Phi_j^{n+1} &= \Phi_j^n + \tau\Pi_j^n \\ \Pi_j^{n+1} &= \Pi_j^n + \tau\left[\frac{\Phi_{j+1}^{n+1} - 2\Phi_j^{n+1} + \Phi_{j-1}^{n+1}}{h^2} + f(\Phi_j^{n+1})\right] \end{aligned} \tag{24}$$

where $\Delta t = \tau$ and $\Delta x = h$; Φ_j^n and Π_j^n are the field operators at the point $(t = n\tau,\ x = jh)$. Schemes (23) and (24) were proposed by Vázquez. The scheme of order 4 constructed by the composition of (23) and (24) is the scheme that appeared in ref. 14.

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