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General theory of higher-order decomposition of exponential operators and symplectic integrators

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A general scheme for a higher-order decomposition of exponential operators and symplectic integrators is constructed and its mathematical structure is clarified using the free Lie algebra and the associated Witt formula. The minimal form of the decomposition is found, and the number of its minimal products is given generally using the Möbius function. An infinite number of recursive schemes are also proposed.

In quantum statistical physics, the so-called Trotter formula [1–3] has been frequently used. The present author [2,3] has extended it to propose a general scheme of quantum Monte Carlo simulations [4,5].

Our generalized Trotter-like formula is expressed by [3,6,7]

$$\exp\left(x \sum_{j=1}^{q} A_j\right) = [f_m(\{A_j/n\})]^n + O(x^{m+1}/n^m) \tag{1}$$

for the mth approximant $f_m(\{A_j\})$ defined in the form

$$\exp\left(x \sum_{j=1}^{q} A_j\right) = f_m(\{A_j\}) + O(x^{m+1}) . \tag{2}$$

As is well known, the first approximant $f_1(\{A_j\})$ corresponding to the Trotter formula is given by

$$f_1(\{A_j\}) = \exp(xA_1)\exp(xA_2)\ldots\exp(xA_q) , \tag{3}$$

and the second approximant $f_2(\{A_j\})$ is given by the following symmetric decomposition [3],

$$f_2(\{A_j\}) \equiv S(x) = \exp(\tfrac{1}{2}xA_1)\ldots\exp(\tfrac{1}{2}xA_{q-1})\exp(xA_q)\exp(\tfrac{1}{2}xA_{q-1})\ldots\exp(\tfrac{1}{2}xA_1) . \tag{4}$$

The above symmetry is characterized [3] by

$$S^{-1}(x) = S(-x) \qquad \text{or} \qquad S(x)S(-x) = 1 . \tag{5}$$

Now, the purpose of the present paper is to construct a general scheme [6–8] to find any higher-order decomposition $f_m(\{A_j\})$ for arbitrary non-commutable operators $\{A_j\}$. In fact, there exists such a scheme. The present author has already proposed a recursive scheme to construct explicitly a higher-order decomposition. Namely the mth approximant $Q_m(x)$ is constructed [6,7] recursively by

$$Q_m(x) = \prod_{j=1}^{r} Q_{m-1}(p_{mj}x) , \tag{6}$$

with the condition that

$$\sum_{j=1}^{r} p_{mj}^{m}=0, \qquad \sum_{j=1}^{r} p_{mj}=1 . \tag{7}$$

However, the number of products of exponential operators such as (4) becomes very large as the parameter m increases. Then there arises the question what is the minimal decomposition. To answer this question, we propose here a general scheme of higher-order decomposition by using Kubo's symmetrization operation S defined by [9]

$$S(x^p y^q)=\frac{p!q!}{(p+q)!}\sum_{\mathrm{P}_m} \mathrm{P}_m(x^p y^q) , \tag{8}$$

where the operation P_m means permutation of the order of the operators x and y in all possible ways. We also use the "time-ordering" operation P introduced in our previous paper [7]:

$$\begin{aligned} P(x_{mj}x_{nk}) &= x_{mj}x_{nk}, \qquad \text{for } j<k , \\ &= x_{nk}x_{mj}, \qquad \text{for } k<j , \end{aligned} \tag{9}$$

for $\{x_{mj}\}$ defined by (13).

First we explain a general scheme for the mth order decomposition in terms of the first-order approximant $Q_1(x)=f_1(\{A_j\})$ as

$$f_m(\{A_j\})=\prod_{j=1}^{r} Q_1(p_j x) . \tag{10}$$

Our main problem is to find some appropriate conditions so that eq. (10) may satisfy eq. (2). If we apply an elementary procedure to find them, then it requires extremely complicated lengthy calculations [6,7,10–15] [#1]. Thus, we propose here an alternative abstract and compact procedure [8]. The approximant $Q_1(x)$ is expressed as

$$Q_1(x)=\exp[x(A_1+\ldots+A_q)+x^2x_2+x^3x_3+\ldots] , \tag{11}$$

where x_n denotes a function of commutators of the operators $\{A_j\}$, namely $x_n=x_n(\{A_j\})$. Then we may write

$$f_m(\{A_j\})=\prod_{j=1}^{r} \exp(x_{1j}+x_{2j}+x_{3j}+\ldots) , \tag{12}$$

where

$$x_{nj}=(p_j x)^n x_n, \qquad x_1=A_1+A_2+\ldots+A_q . \tag{13}$$

Thus, using the time-ordering operation P with respect to the subscript j in (12), we obtain

$$f_m(\{A_j\})=P\exp\left(\sum_j (x_{1j}+x_{2j}+x_{3j}+\ldots)\right)=P\exp(X_1+X_2+X_3+\ldots) , \tag{14}$$

with $X_n=\sum_j x_{nj}$. Using Kubo's symmetrization operation S with respect to operators with the same subscript j, we can write

$$f_m(\{A_j\})=PS(\exp(X_1)\exp(X_2)\exp(X_3)\ldots)=\sum_{n_1,n_2,n_3,\ldots}\frac{1}{n_1!n_2!n_3!\ldots}PS(X_1^{n_1}X_2^{n_2}X_3^{n_3}\ldots) . \tag{15}$$

This is a quite convenient general expression of the mth approximant containing the parameters $\{p_j\}$ which

[#1] The basic formulae in ref. [13] had been published in ref. [6], before ref. [13] had been submitted.

should be determined so that the higher-order correction terms up to the mth order coming from x_2, x_3, ..., and x_m in (15) should vanish. Thus, we have the conditions that

$$PS(X_1^{n_1} X_2^{n_2} \dots) = 0 , \tag{16}$$

for all non-negative integers n_1, n_2, ... under the restriction that $n_1 + 2n_2 + \dots \leqslant m$, excluding $n_2 = n_3 = \dots = 0$.

There are many redundant conditions in (16), and thus we try to select the minimal independent conditions and to estimate the number of such minimal conditions. This is also practically important.

For this purpose, following Kubo [9] we introduce the concept of "cumulant operators" as follows. First we define the following moment operators,

$$\mu_m = \sum_{\substack{n_1, n_2, n_3, \dots \\ \{n_1 + 2n_2 + 3n_3 + \dots = m\}}} \frac{m! x^{-m}}{n_1! n_2! n_3! \dots} PS(X_1^{n_1} X_2^{n_2} X_3^{n_3} \dots) . \tag{17}$$

It should be noted that these moments are operators composed of the original operators $(x_1, x_2, ..., x_m)$ which are defined in (11) and (13). Now the cumulant operators are introduced by the definition

$$\exp\left(\sum_{m=1}^{\infty} \frac{x^m}{m!} \Phi_m \right) = \sum_{m=0}^{\infty} \frac{x^m}{m!} \mu_m . \tag{18}$$

If $\{\mu_m\}$ are c-numbers, then the cumulant κ_m defined by Φ_m in (18) is given by the following formula [16],

$$\kappa_m = (-1)^{m-1} \begin{vmatrix} \mu_1 & 1 & 0 & \dots & & & \\ \mu_2 & \mu_1 & 1 & 0 & & & \\ \mu_3 & \mu_2 & \binom{2}{1}\mu_1 & 1 & 0 & & \\ \mu_4 & \mu_3 & \binom{3}{1}\mu_2 & \binom{3}{2}\mu_1 & 1 & 0 & \\ \mu_5 & \mu_4 & \binom{4}{1}\mu_3 & \binom{4}{2}\mu_2 & \binom{4}{3}\mu_1 & 1 & 0 \\ \vdots & & & & & & \ddots \end{vmatrix}_m , \tag{19}$$

where $\binom{n}{m} = {}_nC_m$. This is also expressed as [9,17]

$$\kappa_m = -m! \sum_{j=1}^{m} \sum_{k_1, k_2, \dots} \left(\sum k_i - 1 \right)! (-1)^{\Sigma k_i} \prod_{i=1}^{j} \frac{1}{k_i!} \left(\frac{\mu_{m_i}}{m_i!} \right)^{k_i} , \tag{20}$$

under the condition that

$$k_1 m_1 + k_2 m_2 + \dots + k_j m_j = m, \qquad \text{for } m_1 < m_2 < \dots < m_j . \tag{21}$$

For example, we have [9]

$$\kappa_1 = \mu_1 , \qquad \kappa_2 = \mu_2 - \mu_1^2 , \qquad \kappa_3 = \mu_3 - 3\mu_2\mu_1 + 2\mu_1^3 , \qquad \dots . \tag{22}$$

Now $\{\mu_m\}$ are operators, and consequently we need some appropriate prescription [9]. It is easily shown that the symmetrization operation S with respect to the subscript j of μ_j is

$$\Phi_m = S\kappa_m . \tag{23}$$

For example, from (22), we obtain

$$\Phi_1 = \mu_1 , \qquad \Phi_2 = \mu_2 - \mu_1^2 , \qquad \Phi_3 = \mu_3 - \tfrac{3}{2}(\mu_1\mu_2 + \mu_2\mu_1) + 2\mu_1^3 , \qquad \dots . \tag{24}$$

In general, the mth cumulant Φ_m is expressed in the form

$$\Phi_m = \mu_m - \Phi'_m(\mu_1, \dots, \mu_{m-1}) , \tag{25}$$

namely,

$$\mu_m = \Phi_m + \Phi'_m(\mu_1, ..., \mu_{m-1}) , \tag{26}$$

with $\Phi'(0, ..., 0)=0$.

In general, it is rather easy to calculate the moments (operators) $\{\mu_m\}$ but it is very complicated to find the cumulants (operators) $\{\Phi_m\}$, as seen from the above relations (20) and (23). However, the cumulants (operators) $\{\Phi_m\}$ have a mathematically convenient property. Namely Φ_2, Φ_3, ... are expressed in terms of some linear combinations of commutators of x_1, x_2, x_3, ..., as is easily confirmed from Friedrich's theorem [18] on the free Lie algebra A_0. That is, as is seen from the relation

$$\exp[(p_1x)x_1+(p_1x)^2x_2+...]\exp[(p_2x)x_1+(p_2x)^2x_2+...]\exp[(p_3x)x_1+(p_3x)^2x_2+...]$$
$$=\exp\left(\sum_{m=1}^{\infty}\frac{x^m}{m!}\Phi_m(x_1,x_2,x_3,...,x_m)\right), \tag{27}$$

the mth cumulant $\Phi_m(\{x_j\})$ is expressed as a linear combination of basic Lie elements of degree n $(=n_1+n_2+...)$ in A_0, where $n_1+2n_2+3n_3+...+mn_m=m$.

Thus, we have the following basic theorem in our problem.

Theorem 1. The mth moment operator $M_m(x_1, x_2, ..., x_m)$ defined by

$$M_m(\{x_j\}) = \sum_{\substack{n_1,n_2,... \\ \{n_1+2n_2+...+mn_m=m,\ n_1\neq m\}}}{}' \frac{m!x^{-m}}{n_1!n_2!...}PS(X_1^{n_1}X_2^{n_2}...) \tag{28}$$

is expressed as a linear combination of basic Lie elements of degree n $(=n_1+n_2+...)$ in A_0 under the condition that

$$M_2=M_3=...=M_{m-1}=0 . \tag{29}$$

Equivalently each moment defined by

$$M_{n_1,n_2,...}(\{x_j\})=x^{-(n_1+2n_2+...)}PS(X_1^{n_1}X_2^{n_2}X_3^{n_3}...) \tag{30}$$

is expressed as a linear combination of basic elements exactly of degrees n_1, n_2, n_3, ... in x_1, x_2, x_3, ..., respectively, under the condition (29).

Proof. First note that from (17) and (28) we have

$$\mu_m=M_m(\{x_j\})+x^{-m}PS(X_1^m) . \tag{31}$$

Here we find easily

$$PS(X_1^m)=PS\left(\sum_j x_{1j}\right)^m=\left(\sum_j p_jx\right)^m x_1^m=(xx_1)^m \tag{32}$$

under the condition

$$p_1+p_2+...+p_r=1 . \tag{33}$$

Thus we have

$$f_m(\{A_j\})=\exp[x(A_1+...+A_q)]+\sum_{n=2}^{\infty}\frac{x^n}{n!}M_n(\{x_j\}) . \tag{34}$$

Therefore, under the condition (29) we have

$$f_m(\{A_j\})=\exp[x(A_1+...+A_q)]+\sum_{n=m}^{\infty}\frac{x^n}{n!}M_n(\{x_j\})\,. \tag{35}$$

Then it is shown recursively that the above function (35) should be expressed in the form

$$f_m(\{A_j\})=\exp\left(x(A_1+...+A_q)+\sum_{n=m}^{\infty}\frac{x^n}{n!}\Phi_n(\{x_j\})\right). \tag{36}$$

Thus, we obtain the relation

$$M_m(\{x_j\})=\Phi_m(\{x_j\}) \tag{37}$$

under the condition (29). This yields the proof of theorem 1.

From this theorem, we can answer the question what is the number of minimal products in the form (10). The result is expressed as follows.

Theorem 2. The minimal number $S_m^{(1)}$ of the parameters $\{p_j\}$ for the mth approximant $f_m(\{A_j\})$ in the form (10) with the first-order approximant $Q_1(x)$ is given by

$$S_m^{(1)}=1+N_2^{(1)}+N_3^{(1)}+...+N_m^{(1)}\,, \tag{38}$$

where

$$N_m^{(1)}=\sum_{\substack{n_1,n_2,...\\ \{n_1+2n_2+...+mn_m=m\}}} M(n_1,n_2,...,n_m) \tag{39}$$

and

$$M(n_1,n_2,...,n_m)=\frac{1}{n}\sum_{d/n_p}\mu(d)\frac{(n/d)!}{(n_1/d)!(n_2/d)!\,...}\,. \tag{40}$$

Here the symbol d/n_p denotes all common divisors of n_1, n_2, ..., n_m, and $n_1+n_2+\,...+n_m=n$. The symbol $\mu(d)$ denotes the Möbius function.

Proof. First remember that the Möbius function $\mu(p)$ is defined [17] for all positive integers by $\mu(1)=1$, $\mu(p)=-1$ if p is a prime number, $\mu(p^k)=0$ for $k>1$, and $\mu(bc)=\mu(b)\mu(c)$ if b, c are coprime integers. Then, Witt's formula [18] [#2] on the free Lie algebra yields immediately the result that the number of independent commutators (basic Lie elements) appearing in the moment operator $M_{n_1,n_2,...}(\{x_j\})$ is given by $M(n_1, n_2, ..., n_m)$ in (40). The number of independent basic Lie elements in the mth momentum operator $M_m(\{x_j\})$ is then given by $N_m^{(1)}$ in (39), because we have $M(m, 0, 0, ..., 0)=0$ for $m\geqslant 2$ in (40). Finally the whole condition on the mth approximant $f_m(\{A_j\})$ is given by the requirement that the whole algebra space $\mathrm{S}^{(m)}$ composed of

$$\mathrm{S}^{(m)}=\mathrm{M}_2\oplus\mathrm{M}_3\oplus\,...\oplus\mathrm{M}_m \tag{41}$$

should shrink to a vanishing space. The condition for this requirement is expressed in terms of $N_2^{(1)}+N_3^{(1)}+\,...+N_m^{(1)}$ parameters of $\{p_j\}$. Adding the first condition (33), we arrive at theorem 2.

It is also possible to construct an infinite number of recursive formulae to find the $(m+m')$th approximant in terms of the mth approximant as follows.

[#2] Professor K. Aomoto kindly brought ref. [18] to our attention.

Theorem 3. There exist an infinite number of recursive formulae to construct higher-order decomposition formulae of exponential operators as follows. We consider a typical mth approximant $Q_m(x)$. Then it is expressed in the form

$$Q_m(x)=\exp(xx_1+x^{m+1}x_{m+1}+x^{m+2}x_{m+2}+\ldots)\,, \tag{42}$$

as before. Now, we try to construct the $(m+m')$th approximant as

$$f_{m+m'}(\{A_j\})=\prod_{j=1}^{r} Q_m(p_jx)\,. \tag{43}$$

In the same way as before, we have

$$f_{m+m'}(\{A_j\})=\exp(xx_1)+\sum_{k_1,k_{m+1},\ldots}{}' \frac{x^{k_1+k_{m+1}+\ldots}}{k_1!k_{m+1}!\ldots} M_{k_1,k_{m+1},\ldots}(\{x_j\})\,, \tag{44}$$

where Σ' denotes the summation over k_1, k_{m+1}, ... for

$$k_1+(m+1)k_{m+1}+(m+2)k_{m+2}+\ldots+(m+m')k_{m+m'}>m\,, \tag{45}$$

excluding $k_{m+1}=k_{m+2}=\ldots=0$, and

$$M_{k_1,k_{m+1},\ldots}=x^{-[k_1+(m+1)k_{m+1}+\ldots]}PS(X_1^{k_1}X_{m+1}^{k_{m+1}}X_{m+2}^{k_{m+2}}\ldots)\,. \tag{46}$$

Thus, the condition on $\{p_j\}$ is given by the requirement that $N_{m,m'}$ independent (basic) Lie elements among $M_{k_1,k_{m+1},\ldots}(\{x_j\})$ should vanish, where

$$N_{m,m'}=\sum_{\substack{k_1,k_{m+1},\ldots \\ \{m<k_1+(m+1)k_{m+1}+\ldots+(m+m')k_{m+m'}\leqslant m+m'\}}} M(k_1,k_{m+1},\ldots,k_{m+m'})\,. \tag{47}$$

In the above scheme of decomposition, the parameters $\{p_j\}$ become complex numbers (not real). Some explicit applications of the above theorems will be reported elsewhere.

From a practical point of view, it is more convenient to construct a symmetrized decomposition [3,6]

$$f_{2m-1}(\{A_j\})=S(p_1x)S(p_2x)\ldots S(p_rx)\,, \tag{48}$$

with $p_{r-j}=p_j$. As was pointed out already in previous papers [3,6,7], the symmetric $(2m-1)$th approximant is also correct up to the $(2m)$th order, namely $f_{2m-1}(\{A_j\})=f_{2m}(\{A_j\})$. The symmetric approximant $S(x)$ is expressed [3,6,7,12,15] as

$$S(x)=\exp[x(A_1+\ldots+A_q)+x_3x^3+x_5x^5+\ldots+x_{2m-1}x^{2m-1}+\ldots] \tag{49}$$

only in terms of odd-order operators x_{2m-1}.

Corresponding to theorem 1, the following theorem holds.

Theorem 4. The $(2m-1)$th moment operator $M_{2m-1}(\{A_j\})$ defined by

$$M_{2m-1}(\{x_j\})=\sum_{\substack{n_1,n_3,\ldots \\ \{n_1+3n_3+\ldots+(2m-1)n_{2m-1}=2m-1,\ n_1\neq m\}}}{}' \frac{(2m-1)!x^{-(2m-1)}}{n_1!n_3!\ldots} PS(X_1^{n_1}X_3^{n_3}\ldots) \tag{50}$$

is expressed as a linear combination of basic Lie elements of degree n $(=n_1+n_3+\ldots)$ in A_0 under the condition that

$$M_3=M_5=\ldots=M_{2m-3}=0\,. \tag{51}$$

Equivalently each moment defined by

$$M_{n_1,n_3,\dots}(\{x_j\}) = x^{-(n_1+3n_3+\dots)} PS(X_1^{n_1} X_3^{n_3} \dots) \tag{52}$$

is expressed as a linear combination of basic elements exactly of degrees n_1, n_3, n_5, ... in x_1, x_3, x_5, ..., respectively, under the condition (51).

Corresponding to theorem 2, the following theorem holds.

Theorem 5. The minimal number S_{2m-1} of the parameters $\{p_j\}$ for the $(2m-1)$th approximant $f_{2m-1}(\{A_j\})$ in the form (48) is given by

$$S_{2m-1} = 1 + N_3 + N_5 + \dots + N_{2m-1} , \tag{53}$$

where

$$N_{2m-1} = \sum_{\substack{n_1,n_3,\dots \\ \{n_1+3n_3+5n_5+\dots+(2m-1)n_{2m-1}=2m-1\}}} M(n_1, n_3, n_5, \dots) \tag{54}$$

and $M(n_1, n_3, n_5, \dots)$ is defined by (40).

Corresponding to theorem 3, the following theorem holds.

Theorem 6. The $(2m+2s)$th approximant $f_{2m+2s}(\{A_j\})$ can be constructed recursively from $Q_{2m}(\{x\})$ as

$$f_{2m+2s}(\{A_j\}) = \prod_{j=1}^{r} Q_{2m}(\{p_j x\}) , \tag{55}$$

where the parameters $\{p_j\}$ are determined by the requirement that the moment operators $M_{n_1,n_{2m+1},\dots}(\{x_j\})$ should vanish for all the values of n_1, n_{2m+1}, ..., $n_{2m+2s-1}$ under the condition that

$$2m+1 \leqslant n_1 + (2m+1)n_{2m+1} + \dots + (2m+2s-1)n_{2m+2s-1} \leqslant 2m+2s-1 , \tag{56}$$

excluding $n_{2m+1} = \dots = n_{2m+2s-1} = 0$.

The case $s=1$ was reported in the previous papers by the present author [6,7].

It is rather easy to obtain explicitly the equations to determine the parameters and the minimal number S_{2m-1} in the above symmetric decomposition scheme. For example, we have $N_3=1$, $N_5=2$, $N_7=4$, $N_9=8$, $N_{11}=18$, $N_{13}=34$, $N_{15}=71$, ..., and consequently we have $S_3=2$, $S_5=4$, $S_7=8$, $S_9=16$, $S_{11}=34$, $S_{13}=68$, $S_{15}=139$, ... Note that $r=2S_{2m-1}-1$.

The corresponding equations to determine the parameters $\{p_j\}$ are given as follows.

Third order: $\sum p_k = 1$, $\sum p_k^3 = 0$;

Fifth order: $\sum p_k = 1$, $\sum p_k^3 = 0$, $\sum p_k^5 = 0$, $\sum p_k^3 a_{1k} b_{1k} = 0$;

Seventh order: $\sum p_k = 1$, $\sum p_k^{2n-1} = 0$ for $n = 2, 3, 4$, $\sum p_k^{2n-1} a_{1k} b_{1k} = 0$ for $n = 2, 3$,

$\sum p_k a_{3k} b_{3k} = 0$, $\sum p_k^3 a_{1k}^2 b_{1k}^2 = 0$;

Ninth order: $\sum p_k=1,\quad \sum p_k^{2n-1}=0$ for $n=2,3,4,5,\quad \sum p_k^{2n-1}a_{1k}b_{1k}=0$ for $n=2,3,4$,

$\sum p_k^{2n-1}a_{1k}^2b_{1k}^2=0$ for $n=2,3,\quad \sum p_k^3a_{1k}^3b_{1k}^3=0,\quad \sum p_k^5a_{3k}b_{1k}=0,$

$\sum p_k^3a_{5k}b_{1k}=0,\quad \sum p_k^3a_{3k}b_{1k}^3=0,\quad \sum p_ka_{3k}^2b_{1k}^2=0,\quad \sum p_ka_{3k}b_{3k}=0;$

Eleventh order: $\sum p_k=1,\quad \sum p_k^{2n-1}=0$ for $n=2,3,4,5,6,\quad \sum p_k^{2n-1}a_{1k}b_{1k}=0$ for $n=2,3,4,5$,

$\sum p_k^{2n-1}a_{1k}^2b_{1k}^2=0$ for $n=2,3,4,\quad \sum p_k^{2n-1}a_{1k}^3b_{1k}^3=0$ for $n=2,3,$

$\sum p_k^{2n-1}a_{3k}b_{1k}=0$ for $n=3,4,\quad \sum p_k^{2n-1}a_{3k}^2b_{1k}^2=0$ for $n=2,3,$

$\sum p_k^{2n-1}a_{5k}b_{1k}=0$ for $n=2,3,\quad \sum p_k^3a_{7k}b_{1k}=0,\quad \sum p_k^5a_{3k}b_{3k}=0,$

$\sum p_k^3a_{5k}b_{1k}^3=0,\quad \sum p_ka_{3k}^3b_{1k}=0,\quad \sum p_k^3a_{3k}b_{1k}^5=0,\quad \sum p_ka_{3k}^2b_{1k}^4=0,$

$\sum a_{5k}a_{3k}p_kb_{1k}^2=0,\quad \sum a_{5k}a_{3k}p_kb_{1k}=0,\quad \sum p_ka_{3k}^2a_{1k}b_{1k}^3=0,\quad \sum p_k^3a_{1k}^4b_{1k}^4=0,$

$\sum p_k^{2n-1}a_{3k}b_{1k}^3=0$ for $n=2,3,\quad \sum p_ka_{3k}b_{3k}=0,$ (57)

where

$$a_{nk}=\sum_{j<k}p_j^n+\tfrac{1}{2}p_k^n,\qquad b_{nk}=\sum_{j>k}p_j^n+\tfrac{1}{2}p_k^n. \tag{58}$$

The detailed derivation of the above equations will be published elsewhere [19]. The third-order conditions have been already obtained by several authors [6,7,10–14]. The above fifth- and seventh-order conditions agree (numerically) with those obtained by Yoshida [13]. There exists always, at least, one real solution of the non-linear simultaneous equations (57), as is seen from their symmetry (odd) property.

The present general scheme of higher-order decomposition of exponential operators and symplectic integrators will be useful in quantum statistical physics [2–7,20], molecular physics [14], particle accelerator physics [10–12] and astrophysics [13].

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