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Hybrid exponential product formulas for unbounded operators with possible applications to Monte Carlo simulations

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Abstract

Some new schemes of exponential product formulas are proposed together with a basic theorem. A typical hybrid fourth-order product formula is given by $\exp[-x(A+B)] = S_a(x/3)Q(x)S_b(x/3)Q(x)S_a(x/3) + O(x^5) = Q(x)S_a(x/3)S_b(x/3)S_a(x/3)Q(x) + O(x^5)$, where $S_a(x) = e^{-xA/2}e^{-xB}e^{-xA/2}$, $S_b(x) = e^{-xB/2}e^{-xA}e^{-xB/2}$, and $Q(x) = \exp(-\frac{1}{2}(x/6)^3[B,[A,B]])$.

In previous papers [1–9], some systematic schemes of exponential product formulas have been studied by restricting them into the following form,

$$e^{-x(A+B)} = e^{-t_1 A}e^{-t_2 B}e^{-t_3 A}\dots e^{-t_M A} + O(x^{s+1}). \tag{1}$$

Here the parameters $\{t_j\}$ are proportional to x and they are determined so that the product (1) may express an sth order approximant. These formulas are very useful in quantum mechanics [10] and statistical mechanics [8], because each factor in the right-hand side of (1) can be expressed analytically in most cases and because the quantum effect, namely the noncommutativity effect of A and B, can be treated very accurately using the above product formulas. The quantum effect is one of the most important problems in modern physics, particularly quantum fluctuations, for example, using quantum Monte Carlo simulations [11–18]. In applying formula (1) to quantum mechanics, the sign of $\{t_j/\mathrm{i}x\}$ is irrelevant, because each factor in (1) is unitary for $x = \mathrm{i}t$. However, the negative sign [2] of $\{t_j/x\}$ gives a serious problem, because it is difficult to treat an exponential operator of the form $\exp(tA)$ for $t > 0$ and for a positive unbounded operator A. In fact, there always appears [2] a negative sign in higher-order decompositions for $s \geqslant 3$, if we confine our product formulas in the form (1) with real $\{t_j\}$. The purpose of the present paper is to extend the product formula (1) to more general schemes. One of such generalized schemes is to make use of the complex decomposition [1,2,4,19] in which $\{t_j\}$ are complex. The simplest complex decomposition is given by [1,2,4,19]

$$Q_3(x) = S_a(\lambda x)S_a(\bar{\lambda} x), \tag{2}$$

where $\lambda = \frac{1}{2}(1 \pm \mathrm{i}/\sqrt{3})$ and

$$S_a(x) = e^{-xA/2}e^{-xB}e^{-xA/2}. \tag{3}$$

A fourth-order decomposition of this form is given by [1,2]

$$Q_4(x) = Q_3(\lambda_4 x)Q_3(\bar{\lambda}_4 x), \tag{4}$$

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with $\lambda_4 = (1 + e^{i\pi/4})^{-1}$. Recursively we obtain [1,2]

$$Q_s(x) = Q_{s-1}(\lambda_s x) Q_{s-1}(\bar{\lambda}_s x), \tag{5}$$

where

$$\lambda_s = \left(1 + e^{i\pi/s}\right)^{-1}. \tag{6}$$

Thus, when we rewrite $Q_s(x)$ in the form (1), we find that $\mathrm{Re}(t_j) > 0$ for $x > 0$ and for $s \leqslant 6$. This property is extremely important when A and B are positive but unbounded operators. This has never been pointed out explicitly in the literature. If we put $t_j = x_j + i y_j$ with real x_j and y_j, then we obtain

$$e^{-t_j A} = e^{-x_j A} e^{-i y_j A}. \tag{7}$$

Therefore, we have

$$\| e^{-t_j A} \| \leqslant \| e^{-x_j A} \| \cdot \| e^{-i y_j A} \| \leqslant 1 \tag{8}$$

for $A \geqslant 0$ and for $s \leqslant 6$. Similarly we have $\| e^{-t_k B} \| \leqslant 1$ for $B \geqslant 0$ and for $s \leqslant 6$. Thus, we can construct higher-order contraction product formulas even for positive unbounded operators. Furthermore, we can show [20] the following strong-norm convergence,

$$\lim_{n \to \infty} \| \left[e^{-x(A+B)} - Q_s^n(x/n) \right] \psi \| = 0 \tag{9}$$

for any vector ψ in the domain $\mathscr{D} = \mathscr{D}(A) \cap \mathscr{D}(B)$, when A, B and $A + B$ are non-negative selfadjoint operators, and when $\{Q_s(x)\}$ are given in the above complex form (5) for $s \leqslant 6$. The above decomposition (5) is a hybrid product scheme in the sense that it is a product of contraction generators and unitary operators. If we try to apply the above hybrid scheme to Monte Carlo simulations, then we have a negative-sign problem in the unitary operators $\{e^{-i y_j A}\}$ and $\{e^{-i y_k B}\}$.

Now, we propose here some general schemes of higher-order decomposition including commutators of A and B. The following Zassenhaus formula,

$$e^{-x(A+B)} = e^{-xA} e^{-xB} e^{-x^2[A,B]/2} e^{-x^3[A+2B,[A,B]]/6} \ldots, \tag{10}$$

is well known [21,22]. However, this contains many kinds of commutators. In fact, it contains an infinite number of independent commutators. On the other hand, our general scheme (1) does not include any commutator even for $s \to \infty$. One of the present main ideas is to consider new general schemes based on a *restricted number* of commutators. We may try to include not only commutators but also polynomials of A and B such as A^2, B^2 and $[A, B]^2$ in constructing product formulas. However, we have the following.

Basic theorem. When an exponential operator $e^{-x(A+B)}$ is expressed in the form

$$e^{-x(A+B)} = e^{C_1} e^{C_2} \ldots e^{C_r} + O(x^{s+1}), \tag{11}$$

each C_j takes one of the free Lie elements (namely, A, B, $[A, B]$, $[B, [A, B]]$, $[A, [A, B]]$, $\ldots$). Even if we add nonlinear elements (namely, A^2, B^2, A^3, $[A, B]^2 \ldots$), they do not affect the coefficients of free Lie elements, namely they are irrelevant to the above product scheme (11). In other words, any number of restricted free Lie elements including A and B can be used as bases of (11) for any order s.

The proof of this basic theorem is given by using Friedricks' theorem [21]. Namely, if $\{C_j\}$ in (11) includes nonlinear elements, then the operator $\Phi(\{C_j\})$ defined by

$$e^{C_1} e^{C_2} \ldots e^{C_r} = \exp \Phi\left(\{C_j\}\right) \tag{12}$$

is decomposed into two parts as

$$\Phi\left(\{C_j\}\right) = \Phi_f\left(\{C_j\}\right) + \Phi_n\left(\{C_j\}\right). \tag{13}$$

Here $\Phi_f(\{C_j\})$ is a linear combination of free Lie elements of A and B and $\Phi_n(\{C_j\})$ denotes the remaining part composed of nonlinear elements. The requirement that $\exp \Phi(\{C_j\})$ is of the order of s yields the conditions that

$$\Phi_f\left(\{C_j\}\right) = -x(A + B) + O(x^{s+1}) \tag{14}$$

and

$$\Phi_n\left(\{C_j\}\right) = O(x^{s+1}). \tag{15}$$

Clearly, the above two operators $\Phi_f(\{C_j\})$ and $\Phi_n(\{C_j\})$ are independent of each other and consequently condition (15) is irrelevant to (14). Furthermore, from Friedricks' theorem [21], we find that $\{C_j\}$ in Φ_f are composed only of free Lie elements of A and B, and that $\{C_j\}$ in Φ_n are composed of the remaining nonlinear elements of $\{C_j\}$. Thus, we arrive at the above basic theorem.

The first new scheme based on the above basic theorem is given in the form (11) with

$$C_j = -t_j x \times (A \text{ or } B) \quad \text{or} \quad C_k = -s_k x^2[A, B] \tag{16}$$

for some $\{j\}$ and $\{k\}$ with $t_j > 0$. In this new scheme, it may be possible to determine $\{t_j\}$ in the region $t_j > 0$ by choosing r and $\{s_k\}$ appropriately for any order s. This proposition will be confirmed elsewhere [23].

In fact, a fourth-order product formula in this scheme is given by

$$Q_4(x) = e^{-x^2C}e^{-A/2}e^{-x^2C}e^{-xB}e^{+x^2C}e^{-A/2}e^{+x^2C}, \tag{17}$$

with $C = \frac{1}{24}[A, B]$. This is easily derived by the Baker–Campbell–Hausdorff formula [21]

$$e^Ae^B = \exp\big(A + B + \tfrac{1}{2}[A, B] + \tfrac{1}{12}[A - B, [A, B]] + \dots\big). \tag{18}$$

In fact, we first note

$$e^{-x^2C}e^{-xB}e^{x^2C} = e^{-xB - x^3[B, C] + O(x^5)}. \tag{19}$$

Then, we have

$$Q_2(x) \equiv e^{-xA/2}\big(e^{-x^2C}e^{-xB}e^{x^2C}\big)e^{-xA/2} = e^{-x(A+B)+x^3[A+B,C]+O(x^5)}. \tag{20}$$

Then, we arrive at

$$Q_4(x) = e^{-x^2C}Q_2(x)e^{x^2C} = e^{-x(A+B)} + O(x^5). \tag{21}$$

Here, we have used the theorem that any symmetric decomposition of $(2m-1)$th order is correct up to the $(2m)$th order [2,24].

The above procedure will be extended [23] to higher-order product formulas based on A, B and C.

Next we discuss another contraction scheme of the form (11) with

$$C_j = -t_j x \times (A \text{ or } B) \quad \text{or}$$

$$C_k = -s_k x^3[B, [A, B]] \tag{22}$$

for $t_j > 0$. As is easily seen, the third-order correction in the BCH formula (18) is composed of the two commutators $[A, [A, B]]$ and $[B, [A, B]]$. More generally, the exponential operator $\exp[-x(A+B)]$ is expanded using the Zassenhaus formula (10). By symmetrization [1,2,24], we have

$$e^{-x(A+B)} = e^{-xA/2}e^{-xB/2}e^{-x^3[A+2B,[A,B]]/24} \times e^{-xB/2}e^{-xA/2} + O(x^5). \tag{23}$$

It is more convenient if only one type of the commutator $[B, [A, B]]$ appears in the decomposition, as in a trace approximant of the fourth order [25]. Thus, we try here to construct a fourth-order operator approximant of the form (11) with (22). Direct calculation of it is so complicated that we have to invent a more convenient procedure. From our experience of deriving the previous scheme (21), we first note

$$S_{\mathrm{aba}}(x) \equiv S_{\mathrm{a}}(px)S_{\mathrm{b}}(qx)S_{\mathrm{a}}(px) = e^{-x(2p+q)(A+B)} \exp\big\{x^3\big[2(p^3 - q^3)A + (4p^3 - q^3)B, C\big]\big\} + O(x^5). \tag{24}$$

Here, $C = \frac{1}{24}[A, B]$ and

$$S_{\mathrm{a}}(x) = e^{-xA/2}e^{-xB}e^{-xA/2},$$
$$S_{\mathrm{b}}(x) = e^{-xB/2}e^{-xA}e^{-xB/2}. \tag{25}$$

If we put $p = q = \frac{1}{3}$ in (24), then we obtain

$$S_{\mathrm{aba}}(x) = e^{-x(A+B)} \exp\big(\tfrac{1}{9}x^3[B, C]\big) + O(x^5). \tag{26}$$

Thus, we arrive at our desired product formulas

$$S_4(x) = Q(x)S_{\mathrm{aba}}(x)Q(x) = Q(x)S_{\mathrm{a}}(x/3)S_{\mathrm{b}}(x/3)S_{\mathrm{a}}(x/3)Q(x) \tag{27}$$

or

$$S_4'(x) = S_{\mathrm{a}}(x/3)Q(x)S_{\mathrm{b}}(x/3)Q(x)S_{\mathrm{a}}(x/3), \tag{28}$$

where

$$Q(x) = \exp\big(-\tfrac{1}{2}(x/6)^3[B, [A, B]]\big). \tag{29}$$

The commutator $[B, [A, B]]$ in (29) is simplified [25–27] as

$$[B, [A, B]] = |\nabla V(r)|^2 \geqslant 0, \tag{30}$$

when

$$A = -\tfrac{1}{2}\Delta, \quad B = V(r). \tag{31}$$

Thus, the above fourth-order formulas (27) and (28) are well-defined contraction operators satisfying the norm inequalities

$$\| S_4(x) \| \leqslant 1, \quad \| S_4'(x) \| \leqslant 1 \tag{32}$$

for $x \geqslant 0$.

The above procedure will be extended [23] to the derivation of higher-order product formulas $\{S_{2m}(x)\}$ for $m \geqslant 3$ of the form (11) with (22). It is also possible to construct many other hybrid schemes [23].

Some explicit applications of the present new schemes will be given elsewhere.

References

[1] M. Suzuki, Phys. Lett. A 146 (1990) 319; 165 (1992) 387.
[2] M. Suzuki, J. Math. Phys. 32 (1991) 400.
[3] M. Suzuki, J. Phys. Soc. Japan 61 (1992) 3015.
[4] M. Suzuki, Physica A 191 (1992) 501.
[5] M. Suzuki and T. Yamauchi, J. Math. Phys. 34 (1993) 4892.
[6] M. Suzuki, Proc. Japan Acad. 69, Ser. B (1993) 161.
[7] M. Suzuki, Commun. Math. Phys. 163 (1994) 491.
[8] M. Suzuki, Physica A 205 (1994) 65, and references therein.
[9] H. Yoshida, Phys. Lett. A 150 (1990) 262.
[10] H. de Raedt and K. Michielsen, Comput. Phys. 8 (1994) 600.
[11] M. Suzuki, Prog. Theor. Phys. 56 (1976) 1454.
[12] M. Suzuki, S. Miyashita and A. Kuroda, Prog. Theor. Phys. 58 (1977) 1377.
[13] M.H. Kalos, ed., Monte Carlo methods in quantum problems (Reidel, Dordrecht, 1982).
[14] H. de Raedt and A. Lagendijk, Phys. Rep. 127 (1986) 233.
[15] M. Suzuki, J. Stat. Phys. 43 (1986) 883.
[16] M. Suzuki, ed., Solid state sciences, Vol. 74. Quantum Monte Carlo methods (Springer, Berlin, 1986).
[17] M. Suzuki, Physica A 194 (1993) 432.
[18] M. Suzuki, ed., Quantum Monte Carlo methods in condensed matter physics (World Scientific, Singapore, 1993).
[19] A.D. Bandrauk and H. Shen, Chem. Phys. Lett. 176 (1991) 428.
[20] M. Suzuki, submitted to J. Math. Phys.
[21] W. Magnus, A. Karrass and D. Solitar, Combinatorial group theory (Dover, New York, 1976).
[22] M. Suzuki, Commun. Math. Phys. 51 (1976) 183.
[23] M. Suzuki, to be submitted to J. Math. Phys.
[24] M. Suzuki, J. Math. Phys. 26 (1985) 601.
[25] M. Takahashi and M. Imada, J. Phys. Soc. Japan 53 (1984) 3765.
[26] T. Kato, Perturbation theory for linear operators (Springer, Berlin, 1966).
[27] N. Okazawa, J. Math. Soc. Japan 34 (1982) 677.