FRACTAL DECOMPOSITION OF EXPONENTIAL OPERATORS WITH APPLICATIONS TO MANY-BODY THEORIES AND MONTE CARLO SIMULATIONS

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A new systematic scheme of decomposition of exponential operators is presented, namely $\exp[x(A+B)]=S_m(x)+O(x^{m+1})$ for any positive integer m, where $S_m(x)=e^{t_1A}e^{t_2B}e^{t_3A}e^{t_4B}...e^{t_MA}$. A general scheme of construction of $\{t_j\}$ is given explicitly. The decomposition $\exp[x(A+B)]=[S_m(x/n)]^n+O(x^{m+1}/n^m)$ yields a new efficient approach to quantum Monte Carlo simulations.

In the present paper, we propose a new scheme of decomposition of exponential operators, which will be useful for quantum Monte Carlo simulations, hopefully even in frustrated quantum spin and fermion systems. In previous papers [1,2], we showed that if we define the following approximant $f_m(\{A_j\})$,

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

then we have

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

The previous choice [1,2] of the mth approximant $f_m(\{A_j\})$ was not necessarily practical. Thus, it is essential to find a new general scheme of construction of $f_m(\{A_j\})$. From a practical point of view, we try here to construct the mth approximant of the form

$$f_m(A,B)=e^{t_1A}e^{t_2B}e^{t_3A}e^{t_4B}...e^{t_MA} \tag{3}$$

for the exponential operator $\exp[x(A+B)]$ with real or complex numbers $\{t_j\}$. The above product decomposition (3) is convenient when A and B are the sum of commuting operators, respectively, because the matrix elements of $f_m(A,B)$ can be obtained easily in these situations, and because it is easy to find an equivalent classical lattice corresponding to the trace of $f_m(A,B)$ in (3).

The simplest decomposition of $\exp[x(A+B)]$ is

$$f_1(A,B)=e^{xA}e^{xB}, \tag{4}$$

as is well known. This is of the first order of x. The second order decomposition is given by the following symmetric product [1–3],

$$S(x)=e^{(x/2)A}e^{xB}e^{(x/2)A}. \tag{5}$$

Clearly, we have [1–3]

$$\exp[x(A+B)]=S(x)+O(x^3). \tag{6}$$

Now we try to find the third order decomposition of the form (3). For this purpose, we express $\exp[x(A+B)]$ as

$$\exp[x(A+B)]=\exp[sx(A+B)]\times\exp[(1-2s)x(A+B)]\exp[sx(A+B)]. \tag{7}$$

Our new strategy of construction of decomposition is to substitute the approximant $S(x)$ into each factor in (7) as

$$S_3(x)=S(sx)S((1-2s)x)S(sx), \tag{8}$$

and to determine the parameter s so that the sum of the uncontrollable third order terms in each S in (8) may vanish. This new scheme of construction can be used repeatedly in higher order approximants as

$$S_m(x)=S_{m-1}(s_mx)S_{m-1}((1-2s_m)x)\times S_{m-1}(s_mx), \tag{9}$$

and the parameter s_m can be determined in a similar way.

More explicitly we explain our construction scheme, called decomposition condition, first for the third order approximant (8). Our possible decomposition condition is that both the sum of the third order terms of each exponential operator in (7)

$$\frac{1}{3!}[2s^3+(1-2s)^3]x^3(A+B)^3 \quad (10)$$

and the sum of the third order terms of each S in (8) may vanish, namely we have

$$2s^3+(1-2s)^3=0\,,$$

$$\text{i.e.,}\quad s=\frac{1}{2-\sqrt[3]{2}}=1.35120719195965\ldots . \quad (11)$$

Thus, the simples real decomposition of third order is given explicitly by

$$S_3(x)=\exp(\tfrac{1}{2}sxA)\exp(sxB)\exp[\tfrac{1}{2}(1-s)xA]$$
$$\times\exp[(1-2s)xB]\exp[\tfrac{1}{2}(1-s)xA]$$
$$\times\exp(sxB)\exp(\tfrac{1}{2}sxA)\,, \quad (12)$$

with s in (11). It is easily shown that there exists no real decomposition of third order expressed by the product of five exponential operators. It should be also remarked that the above symmetric decomposition $S_3(x)$ is correct even up to the fourth order of x, as will be shown generally later. For practical applications, a value of s less than unity is more convenient. For this purpose, we consider the following general decomposition,

$$\exp[x(A+B)]=\prod_{j=1}^{r}\exp[xp_j(A+B)]$$
$$=Q_3^{(r)}(x)+\mathrm{O}(x^4)\,, \quad (13)$$

and

$$Q_3^{(r)}(x)=\prod_{j=1}^{r}S(p_jx)\,, \quad (14)$$

with the decomposition condition that

$$\sum_{j=1}^{r}p_j^3=0 \quad\text{and}\quad \sum_{j=1}^{r}p_j=1\,. \quad (15)$$

For any integer r ($\geqslant 3$), eqs. (15) have real roots less than unity. For example, we have the following solution

$$p_1=p_2=\ldots=p_{r-1}=p=\frac{1}{(r-1)-\sqrt[3]{r-1}}\,,$$

$$p_r=1-(r-1)p\,. \quad (16)$$

In fact, we have that $p=0.641951355\ldots$ for $r=4$.

By generalizing the above scheme, we obtain the following fractal decomposition theorem.

Theorem 1 (construction theorem). For the exponential operator $\exp[x(A_1+A_2+\ldots+A_q)]$, we consider the following $(m-1)$th approximant,

$$\exp\left(x\sum_{j=1}^{q}A_j\right)=Q_{m-1}(x)+\mathrm{O}(x^m)\,. \quad (17)$$

Then, the mth approximant $Q_m(x)$ is constructed as follows:

$$Q_m(x)=\prod_{j=1}^{r}Q_{m-1}(p_{m,j}x)\,, \quad (18)$$

where the parameters $\{p_{m,j}\}$ are the solutions of the following decomposition condition:

$$\sum_{j=1}^{r}p_{m,j}^m=0 \quad\text{with}\quad \sum_{j=1}^{r}p_{m,j}=1\,. \quad (19)$$

The proof of this theorem is easily given by considering the following identity,

$$\exp\left(x\sum_{k=1}^{q}A_k\right)=\prod_{j=1}^{r}\exp\left(p_{m,j}x\sum_{k=1}^{q}A_k\right)$$
$$=Q_m(x)+\mathrm{O}(x^{m+1})\,, \quad (20)$$

and substituting the $(m-1)$th approximant $Q_{m-1}(p_{m,j}x)$ in each factor of (20). The decomposition condition (19) is derived from the requirement that the uncontrollable mth order terms in (20) should vanish.

For $r=2$ and $m=3$, we have the following decomposition,

$$Q_3^{(2)}(x)=S(ax)S(\bar{a}x)\,, \quad (21)$$

where $\bar{a}=1-a$ is the complex conjugate of a, and a and $\bar{a}$ are the solutions of the equation

$$3a^2-3a+1=0\,,\quad \text{i.e.,}\quad a=\tfrac{1}{6}(3\pm\sqrt{3}\,\mathrm{i})\,. \quad (22)$$

More explicitly we have

$$Q_3^{(2)}(x)=\exp(\tfrac{1}{2}axA)\exp(axB)\exp(\tfrac{1}{2}xA)$$
$$\times\exp(\bar{a}xB)\exp(\tfrac{1}{2}\bar{a}xA)\,, \qquad (23)$$

with (22) for $q=2$. This third order complex decomposition (23) was found ad hoc by Bandrauk [4]. Next we obtain the fourth order decomposition

$$Q_4^{(2)}(x)=Q_3^{(2)}(p_4x)Q_3^{(2)}(\bar{p}_4x)\,, \qquad (24)$$

with the decomposition condition

$$p_4^4+(1-p_4)^4=0\,, \quad \text{i.e.,} \quad p_4=(1+e^{i\pi/4})^{-1}. \qquad (25)$$

In general, the mth order approximant is recursively given by

$$Q_m^{(2)}(x)=Q_{m-1}^{(2)}(p_mx)Q_{m-1}^{(2)}((1-p_m)x)\,, \qquad (26)$$

with the decomposition condition

$$p_m^m+(1-p_m)^m=0\,, \quad \text{i.e.,} \quad p_m=(1+e^{i\pi/m})^{-1}\,. \qquad (27)$$

Clearly, we have $\frac{1}{2}<|p_m|<1$ for $m\geqslant 2$, and it is easy to show that

$$\lim_{m\to\infty} p_m=\tfrac{1}{2}\,. \qquad (28)$$

Consequently, our infinite product converges to the original operator, namely

$$\lim_{m\to\infty} Q_m^{(2)}(x)=\exp[x(A+B)]\,. \qquad (29)$$

A more mathematical proof in the Banach space will be given elsewhere. There are many other alternative decomposition schemes, as is easily seen from theorem 1 (construction theorem).

For $q=2$, $r=3$ and $m=3$, we have the following decomposition,

$$Q_3^{(3)}(x)=S(px)S((1-p-q)x)S(px)$$
$$=\exp(\tfrac{1}{2}pxA)\exp(pxB)\exp[\tfrac{1}{2}(1-q)xA]$$
$$\times\exp[(1-p-q)xB]\exp[\tfrac{1}{2}(1-p)xA]\exp(qxB)$$
$$\times\exp(\tfrac{1}{2}qxA)\,, \qquad (30)$$

where p and q satisfy the condition

$$p^3+q^3+(1-p-q)^3=0\,. \qquad (31)$$

The above decomposition is a generalization of (12). In fact, the symmetric case $p=q=s$ of (30) reduces to (12).

It should be noted that the general decomposition condition (19) for $r\geqslant 3$ has always real roots for odd m, but only complex roots for even m. However, we fortunately find that our general symmetric decomposition $S_{2m-1}(x)$ of the order $2m-1$ is correct even up to the order $2m$. Namely, we have

$$S_{2m}(x)=S_{2m-1}(x)\,. \qquad (32)$$

The proof was already given essentially by the present author in 1985 [3]. First note that

$$S_{2m-1}(x)S_{2m-1}(-x)=1\,, \qquad (33)$$

for a symmetric decomposition such as (12), as in ref. [3]. Then, we write $S_{2m-1}(x)$ as

$$S_{2m-1}(x)=\exp\left(x\sum_{j=1}^{q}A_j\right)+x^{2m}R_{2m}(\{A_j\})$$
$$+O(x^{2m+1})\,, \qquad (34)$$

where $R_{2m}(\{A_j\})$ is an operator independent of x. From (33), we have

$$\left[\exp\left(x\sum A_j\right)+x^{2m}R_{2m}(\{A_j\})\right]$$
$$\times\left[\exp\left(-x\sum A_j\right)+x^{2m}R_{2m}(\{A_j\})\right]$$
$$=1+O(x^{2m+1})\,. \qquad (35)$$

That is, we get

$$R_{2m}(\{A_j\})\exp\left(-x\sum A_j\right)$$
$$+\exp\left(x\sum A_j\right)R_{2m}(\{A_j\})=O(x)\,. \qquad (36)$$

Therefore, by putting $x=0$ in (36) we arrive at the conclusion

$$R_{2m}(\{A_j\})=0\,, \qquad (37)$$

namely,

$$S_{2m}(x)=S_{2m-1}(x)\,. \qquad (38)$$

Thus, from theorem 1, we obtain an infinite number of real symmetric decompositions of the exponential operator $\exp[x(A+A_2+...+A_q)]$ up to any order of x.

For practical applications to Monte Carlo simulations including the range of large x, it will be more convenient to use the following decomposition,

$$\exp\left(x\sum_j A_j\right)=[S^*_{2m}(x/n)]^n+O(x^{2m+1}/n^{2m}) . \tag{39}$$

Here, $S^*_{2m}(x)$ is the symmetric decomposition

$$\begin{aligned} S^*_{2m}(x)&=S^*_{2m-1}(x)\\ &=[S^*_{2m-3}(p_m x)]^2 S^*_{2m-3}((1-4p_m)x)\\ &\quad\times[S^*_{2m-3}(p_m x)]^2 , \end{aligned} \tag{40}$$

with the first (or second) order symmetrized decomposition [3]

$$\begin{aligned} S^*_1(x)&=S(x)\\ &=\exp(\tfrac{1}{2}xA_1)\exp(\tfrac{1}{2}xA_2)...\\ &\quad\times\exp(\tfrac{1}{2}xA_{q-1})\exp(xA_q)\exp(\tfrac{1}{2}xA_{q-1})...\\ &\quad\times\exp(\tfrac{1}{2}xA_2)\exp(\tfrac{1}{2}xA_1) , \end{aligned} \tag{41}$$

where the parameter p_m is the real solution of the equation

$$\begin{aligned} &4p_m^{2m-1}+(1-4p_m)^{2m-1}=0 ,\\ &\text{i.e.,}\quad p_m=(4-4^{1/(2m-1)})^{-1} . \end{aligned} \tag{42}$$

Clearly, in this scheme of decomposition, we have $\frac{1}{3}<p_m<\frac{1}{2}$ and $|1-4p_m|<1$ for all m ($\geqslant 2$), as shown in table 1 numerically for explicit applications. The fractal structure of this decomposition is shown in fig. 1. Strictly speaking, it is the "transient fractals" introduced by the present author [5].

Thus, the parameters $\{t_j\}$ in (3) are expressed by some fractal product of $\{p_m\}$ in (42). Then, our general decomposition may be called "fractal decomposition" or "fractal path integral". We call this new approach to simulations "fractal time (or temperature) Monte Carlo" (FTMC).

In applying the above general decomposition to quantum Monte Carlo simulations, we also have to be careful about the length of the additional dimension, namely the number of products of partial Boltzmann factors $e^{t_i A}$ and $e^{t_j B}$. It is estimated to be $(2r^{m-1}+1)n$ for the approximant (39) with the r decomposition in (20) for $q=2$, while it is $2n_0$ for the ordinary Trotter decomposition $\exp[x(A+B)]\doteqdot[\exp(xA/n_0)\exp(xB/n_0)]^{n_0}$. At first glance one might consider that our new scheme requires more products than the ordinary one. However, for the same number of products, the accuracy of our new scheme is much better than the ordinary one; namely the former is of the order of x^{2m+1}/n^{2m} from (39), while the latter is of the order of

$$O(x^2/n_0)=O(x^2/nr^{m-1}) . \tag{43}$$

Thus, our new scheme is much better than the ordinary one, when the criterion

$$(rx/n)^{2m-1}\ll r^m \tag{44}$$

is satisfied.

It is also remarked that the present scheme may hopefully be effective in resolving the "negative sign problem", because the distances of path separation are "fractal" even with respect to sign and because only intrinsic non-commutative effects, namely cross terms, are included in higher orders in our new scheme. It should be noted that the present scheme cannot be applied to a diffusion operator, because there exists no inverse exponential diffusion operator. Finally it should be emphasized that our new scheme is particularly useful in studying quantum coherence.

A more detailed formulation of the present method

Table 1
Numerical values of the decomposition parameters $\{p_m\}$; $M=2\times5^{m-1}+1$.

m	Order	M	p_m
2	4	11	0.41449077179437573714235406286 0...
3	6	51	0.37306582773327282477586304107 3...
4	8	251	0.35958464934999225261241734601 8...
5	10	1251	0.35292403344426771680019442658 8...
6	12	6251	0.34895640496224687051090363759 4...
7	14	31251	0.34632412153470655387804228866 5...

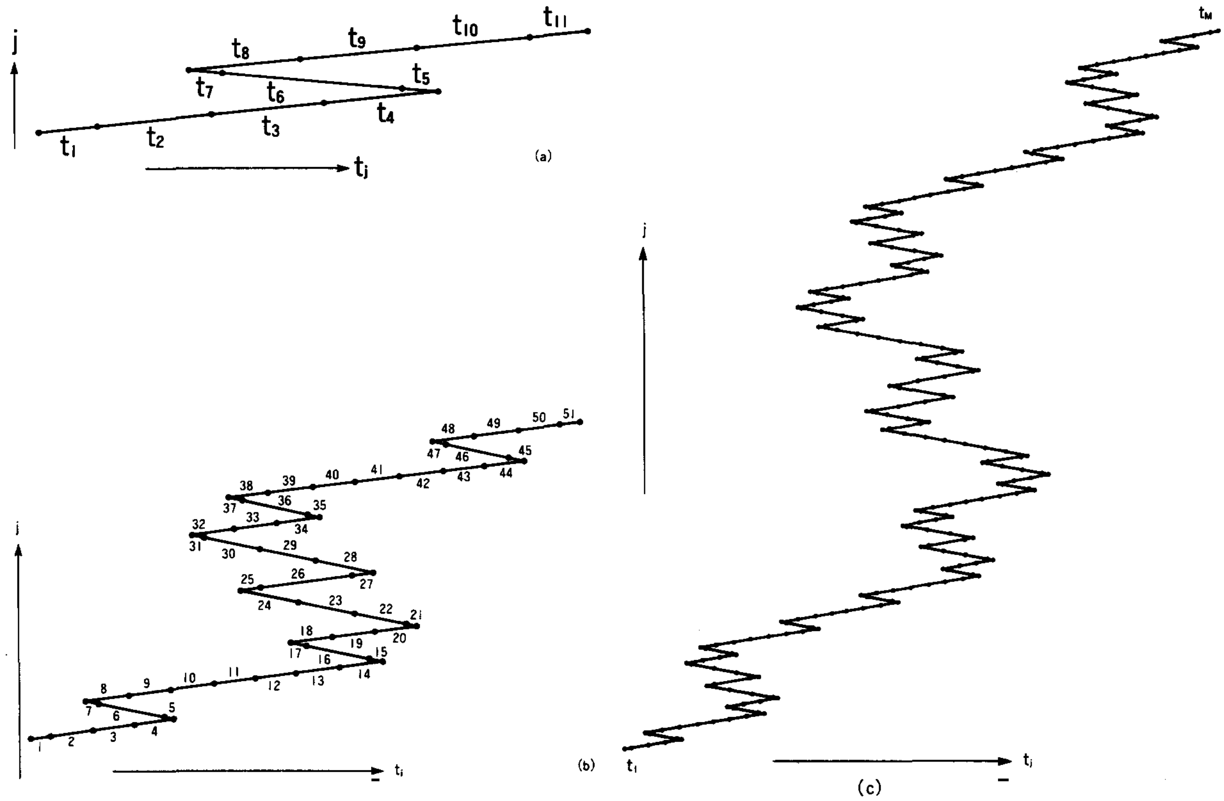

Fig. 1. Fractal structure of the decomposition $S^*_m(x)$: (a) $S^*_3(x)=S^*_4(x)$; $t_1=t_{11}=\frac{1}{2}p_2$, $t_5=t_7=\frac{1}{2}(1-3p_2)$, $t_6=1-4p_2$, others$=p_2$; (b) $S^*_5(x)=S^*_6(x)$: the number j denotes t_j; $t_1=t_{51}=\frac{1}{2}p_2p_3$, $t_5=t_7=t_{15}=t_{17}=t_{35}=t_{37}=t_{45}=t_{47}=\frac{1}{2}(1-3p_2)p_3$, $t_6=t_{16}=t_{36}=t_{46}=(1-4p_2)p_3$, $t_{21}=t_{31}=\frac{1}{2}p_2(1-3p_3)$, $t_{22}=t_{23}=t_{24}=t_{28}=t_{29}=t_{30}=p_2(1-4p_3)$, $t_{25}=t_{27}=\frac{1}{2}(1-3p_2)(1-4p_3)$, $t_{26}=(1-4p_2)(1-4p_3)$, others$=p_2p_3$; (c) $S^*_7(x)=S^*_8(x)$; repeated structure of (b) with the weights p_4, p_4, $1-4p_4$, p_4 and p_4. The four connection distances of five S^*'s are given by $p_2p_3p_4$, $\frac{1}{2}p_2p_3(1-3p_4)$, $\frac{1}{2}p_2p_3(1-3p_4)$ and $p_2p_3p_4$, respectively. In general, $S^*_{2m-1}(x)$ and $S^*_{2m}(x)$ have similar structures. The fractal dimensionality [6] in the limit $m\to\infty$ is given by $D=\log 5/\log 3=1.46\ldots$.

will be reported elsewhere. The present idea of recursive construction of successive approximants may be extended to other approximative methods. Some explicit applications of the present new scheme to Monte Carlo simulations will be reported elsewhere in the near future.

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