# GENERAL CORRECTION THEOREMS ON DECOMPOSITION FORMULAE OF EXPONENTIAL OPERATORS AND EXTRAPOLATION METHODS FOR QUANTUM MONTE CARLO SIMULATIONS

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It is proved that the trace of the generalized Trotter formula $Z(n) \equiv \mathrm{Tr}[\Pi \exp(A_j/n)]^n$ is an even function of $n$, when all $A_j$ are symmetric, namely $A_j^{\mathrm{t}} = A_j$, together with some generalizations. This yields a new extrapolation method of the form $Z(n) \simeq Z(\infty) + a/(n^2+b)$ for large $n$ in quantum Monte Carlo simulations.

In previous papers [1–3] we discussed the convergence of the generalized Trotter formula

$$\exp(A_1 + ... + A_p) = \lim_{n\to\infty} [\exp(A_1/n) \exp(A_2/n) ... \exp(A_p/n)]^n \quad (1)$$

in a Banach space. It was proved in ref. [2] that the trace $Z(n;A,B)$ defined by

$$Z(n;A,B) = \mathrm{Tr}[\exp(A/n)\exp(B/n)]^n \quad (2)$$

is an even function of $n$.

Now we present here some quite general results concerning the convergence of the trace of generalized exponential operators.

We introduce the following general approximants $\{f_{2m}(\{A_j\})\}$ for positive integer $m$:

$$\exp\left(\lambda \sum_{j=1}^{p} A_j\right) = f_{2m}(\{\lambda A_j\}) + O(\lambda^{2m}). \quad (3)$$

Then, we have the following theorem:

*Theorem 1*. If $f_{2m}(\{A_j\})$ satisfies the condition

$$f_{2m}(\{-A_j\})^{-1} = f_{2m}(\{A_j\})^{\mathrm{t}}, \quad (4)$$

then the approximant

$$Z_{2m}(n) \equiv \mathrm{Tr}[f_{2m}(\{A_j/n\})]^n \quad (5)$$

is an even function of $n$, namely

$$Z_{2m}(-n) = Z_{2m}(n). \quad (6)$$

*Proof*. The proof of theorem 1 is quite similar to that of ref. [2]. That is, we have

$$Z_{2m}(-n) = \mathrm{Tr}[f_{2m}(\{-A_j/n\})]^{-n} = \mathrm{Tr}[f_{2m}^{-1}(\{-A_j/n\})]^n = \mathrm{Tr}[f_{2m}(\{A_j/n\})^{\mathrm{t}}]^n = \mathrm{Tr}[f_{2m}^n(\{A_j/n\})]^{\mathrm{t}} = Z_{2m}(n), \quad (7)$$

owing to (4). Theorem 1 yields the following result:

*Theorem 2* (corollary of theorem 1). With the same condition as in theorem 1, we obtain

$$Z_{2m}(n) = Z_{\mathrm{exact}} + O(1/n^{2m}). \quad (8)$$

In particular, if we put [1,2]

$$f_2(\{A_j\}) = \mathrm{e}^{A_1}\mathrm{e}^{A_2} ... \mathrm{e}^{A_p} \quad (9)$$

for symmetric $\{A_j\}$ (namely, $A_j^{\mathrm{t}} = A_j$), then it is easy to confirm that this approximant (9) satisfies the condition (4) of theorem 1 and corresponds to the case $m = 1$ of (3). Thus, we get the following theorem:

*Theorem 3*. If $\{A_j\}$ are symmetric operators (i.e., $A_j^{\mathrm{t}} = A_j$), then we have

$$Z_2(n) \equiv \mathrm{Tr}[\exp(A_1/n)\exp(A_2/n) ... \exp(A_p/n)]^n = Z_2(-n). \quad (10)$$

*Theorem 4* (corollary of theorem 3). With the same condition as in theorem 3, we have

$$Z_2(n) = Z_{\mathrm{exact}} + O(1/n^2). \quad (11)$$

This is nothing but Fye's result [4]. The above theorems are very useful in "quantum statistical Monte Carlo simulations" [5–8].

In practical applications [5–9], the trace $Z_{2m}(n)$ corresponds to the partition function. Now we study the average of any quantum operator $Q$ defined by

$$\langle Q\rangle_m(n) \equiv \mathrm{Tr}\, Q[f_{2m}(\{A_j/n\})]^n / Z_{2m}(n)\,. \qquad (12)$$

Then we have the following theorem:

*Theorem 5.* If $Q$ is a symmetric operator (i.e., $Q^{\mathrm{t}} = Q$) and if the condition (4) is satisfied, then we have

$$\langle Q\rangle_m(-n) = \langle Q\rangle_m(n)\,. \qquad (13)$$

*Proof.* First note the following lemma:

*Lemma.* If $Q$ is symmetric (i.e., $Q^{\mathrm{t}} = Q$), then

$$\mathrm{Tr}\, Q(A^{\mathrm{t}} - A) = 0\,. \qquad (14)$$

The proof of this lemma is given as follows:

$$\mathrm{Tr}\, QA^{\mathrm{t}} = \mathrm{Tr}\, Q^{\mathrm{t}}A^{\mathrm{t}} = \mathrm{Tr}(AQ)^{\mathrm{t}} = \mathrm{Tr}\, AQ = \mathrm{Tr}\, QA\,. \qquad (15)$$

This lemma together with theorem 1 yields

$$\langle Q\rangle_m(-n) = \mathrm{Tr}\, Q[f_{2m}(\{-A_j/n\})]^{-n}/Z_{2m}(-n)$$
$$= \mathrm{Tr}\, Q[f^n_{2m}(\{A_j/n\})]^{\mathrm{t}}/Z_{2m}(n) = \langle Q\rangle_m(n)\,. \qquad (16)$$

*Theorem 6* (corollary of theorem 5). With the same conditions as in theorem 5, we have

$$\langle Q\rangle_1(n) = \langle Q\rangle_{\mathrm{exact}} + \mathrm{O}(1/n^2)\,. \qquad (17)$$

The above results agree with Betsuyaku's results [8] and other numerical ones [9]. Ordinary hamiltonians such as the Heisenberg model satisfy the conditions of the above theorems.

The above theorems suggest the following new extrapolation methods

$$Z_{2m}(n) \quad (\text{or}\ \langle Q\rangle_m(n)) \simeq \frac{1}{n^{2m-2}}\frac{a}{n^2+b} + c\,. \qquad (18)$$

All the traces of higher order symmetrized products introduced in ref. [3] satisfy the condition (4) and consequently are even functions of $n$. The values $a$, $b$ and $c$ can be determined with the use of the least squares method from the numerical data of quantum statistical Monte Carlo simulations [5–8]. The value $c$ gives the desired quantity of the partition function $Z$ (or the average $\langle Q\rangle$).

Some explicit applications of these theorems will be reported somewhere else.

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