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Generalization of the Lie-Trotter Product Formula for q-Exponential Operators

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Abstract

The Lie-Trotter formula $e^{\hat{A}+\hat{B}} = \lim_{N\to\infty}\left(e^{\hat{A}/N}e^{\hat{B}/N}\right)^N$ is of great utility in a variety of quantum problems ranging from the theory of path integrals and Monte Carlo methods in theoretical chemistry, to many-body and thermostatistical calculations. We generalize it for the q-exponential function $e_q(x) = [1+(1-q)x]^{(1/(1-q))}$ (with $e_1(x) = e^x$), and prove $e_q(\hat{A}+\hat{B}+(1-q)[\hat{A}\hat{B}+\hat{B}\hat{A}]/2) = \lim_{N\to\infty}\left\{\left[e_{1-(1-q)N}\left(\hat{A}/N\right)\right]\left[e_{1-(1-q)N}\left(\hat{B}/N\right)\right]\right\}^N$. This extended formula is expected to be similarly useful in the nonextensive situations.

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The Lie-Trotter product formula states that if $\hat{A}$ and $\hat{B}$ are not necessarily commuting finite square matrices or bounded operators with respect to some convenient norm, then

$$e^{\hat{A}+\hat{B}} = \lim_{N\to\infty}\left(e^{\hat{A}/N}e^{\hat{B}/N}\right)^N \ . \tag{1}$$

This formula has been central in the development of path integral approaches to quantum theory, stochastic theory, and in quantum statistical mechanics [1, 2]. In particular, Suzuki has employed this to develop quantum statistical Monte Carlo methods [3, 4], general theory of path integrals with application to many-body theories and statistical physics [5], and more recently to mathematical physics [6]. In the past decade, the use of monomial form of the exponential function [7] defined by (hereafter called q-exponential)

$$e_q(x) = [1+(1-q)x]^{1/(1-q)} \qquad (q \in \mathcal{R}) \tag{2}$$

with a cut-off, for $q < 1$, when $[1 + (1 - q)x] < 0$ (analogously, for $q > 1$, $e_q(x)$ diverges at $x = 1/(q - 1)$), has played an important role in the development of nonextensive statistical physics [8]. Here we consider the corresponding q-exponential operator defined similarly by

$$e_q(\hat{A}) = [1 + (1 - q)\hat{A}]^{1/(1-q)} \qquad (q \in \mathcal{R}) \ . \tag{3}$$

Here, $\hat{A}$ can be a c-number, a square matrix, or an operator. For q going to 1, this goes to the usual exponential form defined in Eq. (1). There is a large class of problems (Levy-like[9] and correlated-like[10] anomalous diffusion, turbulence[11] in nonneutral plasma, nonlinear dynamics[12], solar neutrino problem[13], cosmology[14], electron-positron collisions[15], reassociation of heme-ligands in folded proteins[16], among many others) with a (multi)fractal structure in the relevant space-time in which this and related functional forms emerge naturally. Many of these have received until now only a classical approach; however, their quantum counterparts could be analyzed as well, and then the operator form we are addressing would be the natural one to employ. In this paper, we wish to present the generalization of the formula in Eq. (1) for these monomial functions in the form:

$$e_q(\hat{A} + \hat{B} + (1 - q)\{\hat{A}, \hat{B}\}/2) = \lim_{N\to\infty} \left\{ \left[e_{1-(1-q)N} \left(\hat{A}/N \right) \right] \left[e_{1-(1-q)N} \left(\hat{B}/N \right) \right] \right\}^N \tag{4}$$

where $\{\hat{A}, \hat{B}\} \equiv (\hat{A}\hat{B} + \hat{B}\hat{A})$. Note that $e_{1-(1-q)N}(\hat{A}/N) = [1+(1-q)\hat{A}]^{(1/(1-q)N)}$, has the properties that it goes to $e^{(\hat{A}/N)}$ both when $q = 1$ for finite N and for $q \neq 1$, but $N \to \infty$, so that we recover Eq. (1) appropriately. To establish Eq. (4), we first consider the following pair of operators:

$$\begin{aligned} \hat{C} &= \left[e_{\tilde{q}} \left(\frac{\hat{A} + \hat{B} + (1 - \tilde{q})\{\hat{A}, \hat{B}\}/2N}{N} \right) \right] ; \\ \hat{D} &= e_{\tilde{q}}(\hat{A}/N) e_{\tilde{q}}(\hat{B}/N) \ . \end{aligned} \tag{5}$$

Then, following similar steps as in the case of the exponential operators in [1], the norms of these operators are found to be bounded by the following inequalities:

$$\|\hat{C}\| \leq \left[e_{\tilde{q}} \left(\left\| \frac{\hat{A}+\hat{B}+(1-\tilde{q})\{\hat{A},\hat{B}\}/2N}{N} \right\| \right) \right] \leq \left[e_{\tilde{q}} \left(\frac{\|\hat{A}\|+\|\hat{B}\|+\frac{(1-\tilde{q})}{N}\|\hat{A}\|\|\hat{B}\|}{N} \right) \right] \tag{6}$$

and

$$\begin{aligned} \|\hat{D}\| &\leq \|e_{\tilde{q}}(\hat{A}/N)\| \|e_{\tilde{q}}(\hat{B}/N)\| \\ &\leq e_{\tilde{q}}(\|\hat{A}\|/N) e_{\tilde{q}}(\|\hat{B}\|/N) \\ &= e_{\tilde{q}} \left(\left(\|\hat{A}\| + \|\hat{B}\| + \frac{(1 - \tilde{q})}{N} \|\hat{A}\| \|\hat{B}\| \right) /N \right) \\ &= \left[1 + \frac{(1 - \tilde{q})}{N} \left(\|\hat{A}\| + \|\hat{B}\| + \frac{(1 - \tilde{q})}{N} \|\hat{A}\| \|\hat{B}\| \right) \right]^{(1/(1-\tilde{q}))} \\ &= \left[e_{\tilde{q}} \left(\frac{\|\hat{A}\| + \|\hat{B}\| + \frac{(1-\tilde{q})}{N} \|\hat{A}\| \|\hat{B}\|}{N} \right) \right] \end{aligned} \tag{7}$$

where we have used that (i) the norm of an increasing function of an operator cannot exceed the function of the norm of that operator, (ii) the norm of a sum of two operators cannot exceed the sum of the norms of those operators, and (iii) the norm of the product of two operators cannot exceed the product of the norms of those operators. These expressions are valid for bounded operators as long as the restrictions mentioned after Eq. (2) are obeyed. In the last line in Eq. (7), we used the identity which follows from Eq. (2) for c-numbers, that

$$e_{\tilde{q}}(x)e_{\tilde{q}}(y) = e_{\tilde{q}}(x + y + (1-\tilde{q})xy) \tag{8}$$

in which we set $x = \|\hat{A}\|/N$, and $y = \|\hat{B}\|/N$. Thus the norms of the two operators are found to be bounded by the same quantity. We now calculate the norm $\|\hat{C}^N - \hat{D}^N\|$. We therefore consider the operator identity given in [1, 2],

$$\hat{C}^N - \hat{D}^N = \sum_{k=1}^{N} \hat{C}^{k-1}(\hat{C} - \hat{D})\hat{D}^{N-k} \ , \tag{9}$$

and find a bound on the left side of this equation by the norm on the right hand side, using Eqs. (6) and (7):

$$\begin{aligned} \|\hat{C}^N - \hat{D}^N\| &\leq \sum_{k=1}^{N} \|\hat{C}\|^{k-1}\|(\hat{C} - \hat{D})\|\|\hat{D}\|^{N-k} \\ &\leq N\|(\hat{C} - \hat{D})\| \left[1 + \frac{(1-\tilde{q})}{N}\left(\|\hat{A}\| + \|\hat{B}\| + \frac{(1-\tilde{q})}{N}\|\hat{A}\|\|\hat{B}\|\right)\right]^{((N-1)/(1-\tilde{q}))} \end{aligned} \tag{10}$$

Expanding $\hat{C}$ and $\hat{D}$ in a power series in $(1/N)$, we now estimate the norm of their difference for large N

$$\begin{aligned} \| \, (\hat{C} - \hat{D}) \, \| &\leq \left\| \begin{array}{l} \left(\begin{array}{l} 1 + \left[\frac{\hat{A}+\hat{B}+(1-\tilde{q})\left\{\hat{A},\hat{B}\right\}/2N}{N}\right] \\ +\frac{\tilde{q}}{2}\left[\frac{\hat{A}+\hat{B}+(1-\tilde{q})\left\{\hat{A},\hat{B}\right\}/2N}{N}\right]^2 + \ldots \end{array} \right) \\ -\left(1 + \left[\frac{\hat{A}}{N}\right] + \frac{\tilde{q}}{2}\left[\frac{\hat{A}}{N}\right]^2 + \ldots\right)\left(1 + \left[\frac{\hat{B}}{N}\right] + \frac{\tilde{q}}{2}\left[\frac{\hat{B}}{N}\right]^2 + \ldots\right) \end{array} \right\| \\ &\leq \frac{1}{2N^2} \, \| \left[\hat{A}, \hat{B}\right] + o(\frac{1-\tilde{q}}{N^3}) \, \|, \end{aligned} \tag{11}$$

where $[\hat{A}, \hat{B}] \equiv \hat{A}\hat{B} - \hat{B}\hat{A}$. It is worth noticing that there is no $1/N$ term.
By using inequality (11) into (10) we have thus obtained the following inequality for any $\tilde{q}$ and large N:

$$\|\hat{C}^N - \hat{D}^N\| \leq \frac{1}{2N}\|[\hat{A}, \hat{B}]\| \left[1 + \frac{(1-\tilde{q})}{N}\left(\|\hat{A}\| + \|\hat{B}\| + \frac{(1-\tilde{q})}{N}\|\hat{A}\|\|\hat{B}\|\right)\right]^{((N-1)/(1-\tilde{q}))} . \tag{12}$$

We now let $\tilde{q} = 1 - (1-q)N$, which implies $o(\frac{1-\tilde{q}}{N^3}) = o(1/N^2)$, and take the limit $N \to \infty$, thus showing that the right side of Eq. (12) tends to zero, which implies the required generalization of the Lie-Trotter formula, Eq. (4), i.e.,

$$\{1 + (1-q)[\hat{A} + \hat{B} + (1-q)\{\hat{A}, \hat{B}\}/2]\}^{\frac{1}{1-q}} = lim_{N\to\infty}\{[1 + (1-q)\hat{A}]^{\frac{1}{(1-q)N}}[1 + (1-q)\hat{B}]^{\frac{1}{(1-q)N}}\}^N \tag{13}$$

In conclusion, we have generalized here (Eq. (4) or, equivalently, Eq. (13)) the Lie-Trotter formula, for q-exponential operators which occur in the development of nonextensive statistical physics[8]. It is expected that this formula will be useful in quantum versions of generalized simulated annealing[17] and in accelerating the rate of convergence of algorithms used in quantum chemistry[4], as well as for performing calculations of quantum nonextensive systems.

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