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Tomaž Prosen and Iztok Pižorn

Physics Department, Faculty of Mathematics and Physics, University of Ljubljana, Jadranska 19, SI-1000 Ljubljana, Slovenia

Abstract
We propose a high order numerical decomposition of exponentials of Hermitian operators in terms of a product of exponentials of simple terms, following an idea which has been pioneered by M Suzuki, implementing it for complex coefficients. We outline a convenient fourth-order formula which can be written compactly for an arbitrary number of non-commuting terms in the Hamiltonian and which is superior to the optimal formula with real coefficients, both in complexity and accuracy. We show asymptotic stability of our method for a sufficiently small time step and demonstrate its efficiency and accuracy in different numerical models.

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1. Introduction

While exponentials of operators are very common not only in every field of quantum physics, but also in classical physics, their evaluation is nevertheless numerically a very demanding operation. For example, in quantum physics, this task usually emerges when one wants to compute a time evolution, either in real time, for example, when computing dynamical correlations, or in imaginary time, when computing thermodynamic averages such as in quantum Monte Carlo simulations. A similar decomposition of classical time evolution, which can also be interpreted in terms of unitary operators, is known as symplectic integration.

For an operator which can be written as a sum of several parts of which exponential operators are exactly determinable, the well-known Suzuki–Trotter [1–7] decomposition scheme can be used. The operator $e^{iz \sum_j A_j}$ is approximated by a product of operators $e^{iz p_{k_j} A_j}$ with *real* coefficients p_k such that the desired order of accuracy is achieved. We will show in the present paper that following the same principles but not restricting to real coefficients, the same order can be achieved using a smaller number of factors. Furthermore, the order of such a decomposition can be trivially increased by one by composing it with an equivalent

decomposition with a complex conjugate set of coefficients. We will outline a particular third-order scheme, and further improve to fourth order, which is potentially very useful for practical calculations. We show explicitly that, even though we lose unitarity of decomposition (in a real-time case), the method is asymptotically stable for sufficiently small time steps since all the eigenvalues of the decomposition remain on the complex unit circle. Even more generally, we show that one gains an extra order in accuracy and asymptotic stability (independent of the size of the time step) by renormalizing the state vector after each time step.

We demonstrate the accuracy and efficiency of the method by three explicit examples: (i) in the case of 2×2 matrices, the decomposition and its stability can be treated analytically; (ii) for exponentials of Gaussian random Hermitian matrices, we find that the stability threshold (the maximal time step for which the method is asymptotically stable) drops with the inverse power of the dimension of the matrix and (iii) for a generic (non-integrable) interacting spin-$1/2$ chain (in one dimension) we find, surprisingly, that the stability threshold is independent of the number of spins.

2. Complex split-step decomposition

Our main objective is to approximate the exponential operator $U_0 = e^{iz(A+B)}$, for general bounded operators A and B, and a complex parameter z, as a product U of the exponential operators

$$e^{iz(A+B)} = e^{izp_1 A} e^{izp_2 B} e^{izp_3 A} e^{izp_4 B} e^{izp_5 A} + \mathcal{O}(z^4).$$ (1)

We stress again that A and B should be chosen such that, if possible, the action of the exponentials e^{izA} and e^{izB} can be easily calculated (e.g. diagonal operators in simple bases such as position or momentum bases in quantum mechanics). The equations determining the coefficients $\{p_j\}$ that solve the equation above are obtained by expanding the exponential operators into power series and equating the lowest order terms to zero. It is known that there is no third-order ($\mathcal{O}(z^4)$) solution of the five-term ansatz (1) with real coefficients p_j. The simplest third-order decomposition involves six terms [5]. However, allowing the coefficients p_j to be complex, there exist *two* very simple and symmetric solutions, namely[1]

$$p_1 = \overline{p_5} = \frac{1}{4} + \frac{\sqrt{3}}{12}i, \qquad p_2 = \overline{p_4} = \frac{1}{2} + \frac{\sqrt{3}}{6}i, \qquad p_3 = \frac{1}{2}$$ (2)

and the complex conjugate set $\{\overline{p_j}\}$.

Let us denote an exact exponential as $U_0(z) = \exp(iz(A + B))$ and third-order complex decompositions (C3), given by the rhs of (1) with coefficients (2), namely $\{p_j\}$ and $\{\overline{p_j}\}$, as $U(z)$ and $\overline{U}(z)$, respectively. Using some further analysis (which has been performed by means of Mathematica software), we can show that the next-order term changes sign when one switches between the two solutions, namely

$$U(z) = U_0(z) + K_4 z^4 + \mathcal{O}(z^5) \qquad \text{and} \qquad \overline{U}(z) = U_0(z) - K_4 z^4 + \mathcal{O}(z^5),$$ (3)

where

$$K_4 = \frac{i}{144\sqrt{3}}((AAAB - BAAA) - 3(AABA - ABAA) - 3(AABB - BBAA)$$
$$+ 6(ABAB - BABA) + 2(ABBB - BBBA) + 6(BABB - BBAB))$$ (4)

is a Hermitian operator provided that both A and B are Hermitian.

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[1] It was quoted in [6] that this solution had already been proposed by AD Bandrauk; however, it was claimed in [8] that the complex coefficient decomposition is unstable and cannot be practically used for splitting the unitary exponentials, which we show is not precise.
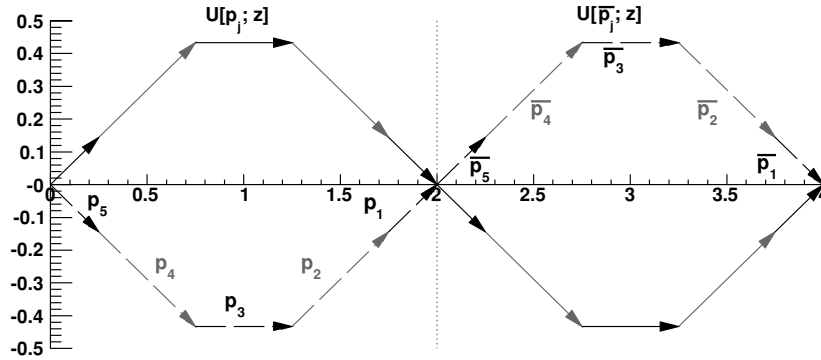
Figure 1. Schematic illustration of complex-valued split-step decomposition. The coefficients p_j can be considered as shifts in complex time plane, which always move along the real axis. Two sets of complex coefficients $\{p_i\}$ give a third-order decomposition $\mathcal{O}(z^4)$; their superposition is for an order higher.

Superposition of the two decompositions cancels the z^4 term and is therefore for one-order higher, namely of fourth order. However, the same fourth order can be achieved by alternating both decompositions (as illustrated in figure 1)

$$\overline{U}(z)U(z) = U_0^2 + (U_0 K_4 - K_4 U_0)z^4 + \mathcal{O}(z^5) = U_0^2 + \mathcal{O}(z^5), \quad (5)$$

since $U_0(z) = 1 + \mathcal{O}(z)$. Since in usual numerical simulations of exponential operators, for example, in quantum time evolutions, time-dependent renormalization group methods or quantum Monte Carlo simulations, one needs to make many time steps anyway, the alternation between $U(z)$ and $\overline{U}(z)$ does not represent any practical drawback.

However, we note that with p_i being complex numbers, the decomposition $U(z)$ is no longer *strictly unitary* (in the usual case where the operators A and B are Hermitian and the time step z is real) and the time evolved state (on which U operates) might explode in norm after a while. In order to strictly preserve the norm, the state (vector) may be renormalized at every time step. One might be afraid that this renormalization would degrade the accuracy of the method. However, due to the fact $K_4^\dagger = K_4$ this is not the case; in fact, renormalization *increases* the accuracy to the fourth order

$$\frac{\langle U_0^\dagger(z)U(z)\rangle}{\sqrt{\langle U^\dagger(z)U(z)\rangle}} = \frac{1 + \langle K_4\rangle z^4 + \mathcal{O}(z^5)}{\sqrt{1 + \langle K_4 + K_4^\dagger\rangle z^4 + \mathcal{O}(z^5)}} = 1 + \mathcal{O}(z^5). \quad (6)$$

By $\langle \cdot \rangle := \langle \psi | \cdot | \psi \rangle$ we denote the expectation value in some intial state vector $| \psi \rangle$. In conclusion, the decomposition with one single set of complex coefficients p_i (C3) is already of the fourth order ($\mathcal{O}(z^5)$) if every time step is followed by renormalization of the state (figure 2). As in any application, the computational complexity of performing the sequence of exponential operators on a state vector $U(z)|\psi\rangle$ is dominating the normalization of the state, this does not represent any drawback of the method. Still, as we will show later, the method is asymptotically stable, for sufficiently small z even without the renormalization. Figure 2 shows real numerical errors in a model in which A and B are chosen as Gaussian random Hermitian matrices, after performing two time steps with various decompositions described above (using one (C3) or both sets of complex coefficients (C4), and with or without the renormalization of the state) and compare it with the optimal third-order decomposition with real coefficients (R3).
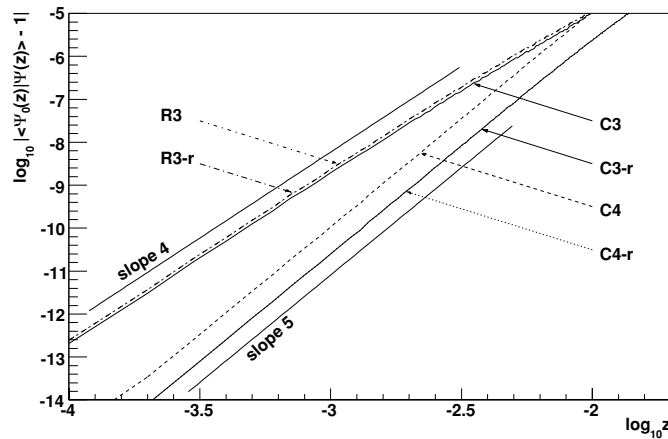
Figure 2. An error after two time steps for the third-order real decomposition (R3), the third-order complex decomposition (C3) and the fourth-order complex decomposition (C4); the label 'r' denotes renormalization after each time step. As for the numerical model, we choose A and B to be GUE matrices of dimension $N = 200$ and average the results over 1000 realizations. We note that renormalization does not change the accuracy in the unitary case with real coefficients; hence, the curves (R3) and (R3-r) are practically the same.

We can easily generalize our approach to approximate exponentials of three or more non-commuting bound operators. For example, for three operators, one has nine terms following a sequence $ABCBABCBA$ which is obtained from $ABABA$ (1) by replacing each inner operator B by BCB (and dividing the coefficient in front of B by two)

$$e^{iz(A+B+C)} = e^{izp_1A} e^{izp_1B} e^{izp_2C} e^{izp_1B} e^{izp_3A} e^{izp_4B} e^{izp_5C} e^{izp_4B} e^{izp_5A} + \mathcal{O}(z^4), \tag{7}$$

and using the same set of coefficients (2), or its complex conjugate. Generally, a formula for a sum of n operators involves $4n - 3$ terms

$$\exp(iz(A_1 + \cdots + A_n)) = e^{izp_1A_1} e^{izp_1A_2} \cdots e^{izp_1A_{n-1}} e^{izp_2A_n} e^{izp_1A_{n-1}} \cdots e^{izp_1A_2}$$
$$\times e^{izp_3A_1} e^{izp_5A_2} \cdots e^{izp_5A_{n-1}} e^{izp_4A_n} e^{izp_5A_{n-1}} \cdots e^{izp_5A_2} e^{izp_5A_1}. \tag{8}$$

It is interesting to note that the general optimal third-order solution with real coefficients (R3) uses just one term more for the case $n = 2$, namely six, whereas for a general n case it needs $5n - 4$ terms, which is $n - 1$ terms more than the complex solution above (8).

As we have mentioned before, without the renormalization complexity of the coefficients may cause the exponential instability of the method. However, it turns out that the decomposition is absolutely stable for enough small steps z. The reason for such an interesting behaviour is that all the eigenvalues of the operator $U(z)$ lie on a complex unit circle for sufficiently small z, and this property grants the asymptotic stability even if $U(z)$ is not exactly unitary. There is typically a threshold, i.e. a critical value of $z_{\max}$ such that at $z = z_{\max}$ two eigenvalues of $U(z)$ collide and leave the unit circle and then the method ceases to be asymptotically stable. Such a behaviour can be explicitly proven for operators chosen from the space of 2×2 matrices (see the following section) and is conjectured in general.

3. Examples

First, let us consider a numerical example of calculating the exponential of $H = A + B$ where A and B are Gaussian random Hermitian matrices chosen at random from the Gaussian unitary
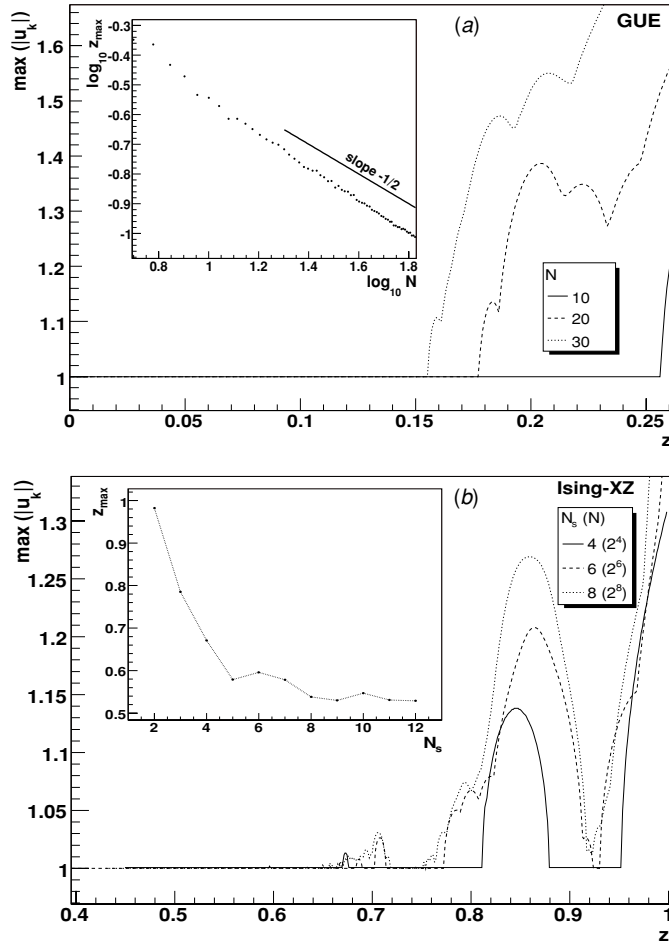
Figure 3. The maximal size of the eigenvalue of the approximate evolution operator $U(z)$. The upper plot (a) shows the case of GUE matrices while the lower plot (b) shows the case of Ising spin chain in a tilted magnetic field (see text). The different curves refer to systems of different sizes (b), or different matrix dimensions (a). The insets show critical threshold z_{max} as a function of the system size/matrix dimension.

ensemble [9]. We note that this example is only meant as a benchmark for presumably the worst case performance of the method and does not provide any practical gain since calculating the exponentials of A and B is not easier than calculating the exponential of H. Figure 3(a) shows that the maximal size of the eigenvalue of $U(z)$ is exactly equal to 1 until some point described by the threshold step size z_{max}. Numerical results suggest the following dependence of the threshold on the Hilbert space dimension N, $z_{max} \propto 1/N^{\alpha}$, with $\alpha \approx 0.5$, which we believe is the worst case scenario for generic systems.

As a second example, we consider a non-trivial physical model where the matrices of the operators A and B are very sparse and thus far from the full random matrix model, namely, we consider time evolution in the quantum Ising spin $1/2$ chain in a tilted homogeneous magnetic field (e.g. recently considered in the context of heat transport [10]) described by the Hamiltonian $H = \sum_{n=1}^{N} \left\{ -J\sigma_n^z \sigma_{n+1}^z + g_x \sigma_n^x + g_z \sigma_n^z \right\}$. Here, $\sigma_n^{x,y,z}$, $n = 1, \ldots, N_s$, represent

a set of independent Pauli matrices. In figure 3(b) we show a very interesting result for this model (in particular, for the parameter values $J = 1, g_x = 0.4, g_z = 0.8$ which lie in the so-called quantum chaotic regime [10]), namely that the threshold step size z_{max} is asymptotically independent of the size $N = 2^{N_s}$ of the system. We conjecture that this is in general true for numerical simulations of finite (spin) quantum systems with local interaction, and as such our method of simulation of time evolution should be very robust. As for the last example, we make analytical consideration of the simplest case where our operators can be represented by 2×2 matrices. In order to understand the transition in the stability (collision of eigenvalues of $U(z)$ on the unit circle), one can generally parametrize the operators A and B by Pauli operators σ^j, $j = 1, 2, 3$,

$$A = a_0 1 + \sum_{j=1}^{3} a_j \sigma^j \qquad \text{and} \qquad B = b_0 1 + \sum_{j=1}^{3} b_j \sigma^j. \tag{9}$$

The coefficients $\{a_j\}$ and $\{b_j\}$ are all real since the matrices A and B are Hermitian, and furthermore, the matrices A and B can always be chosen traceless by setting $a_0 = b_0 = 0$ without losing generality. It is obvious that since $\det U = e^{iz \text{Tr} H}$, where $H = A + B$, that decomposition (1) for two 2×2 matrices can also be expressed in terms of Pauli matrices and some coefficients $\{g_j\}$. Using the ansatz (1), we write

$$e^{izp_1 \sum_j a_j \sigma^j} e^{izp_2 \sum_j b_j \sigma^j} e^{izp_3 \sum_j a_j \sigma^j} e^{izp_4 \sum_j b_j \sigma^j} e^{izp_5 \sum_j a_j \sigma^j} = e^{iz \sum_j g_j \sigma^j}. \tag{10}$$

Of course, g_j are no longer real in general. The eigenvalues of the operator $U(z) = e^{iz \sum_j g_j \sigma^j}$ are $e^{\pm iz \sqrt{\sum_j g_j^2}}$, which give the condition for the asymptotic stability: namely, the number $\gamma^2 = \sum_j g_j^2$ should be *real* and *positive*, $\gamma^2 \in \mathbb{R}^+$. In order to simplify the notation, let us take $\gamma = +\sqrt{\sum_j g_j^2}$ and similarly write $\alpha = \sqrt{\sum_j a_j^2}, \beta = \sqrt{\sum_j b_j^2}$, and introduce normalized coefficients $\gamma_i = g_i/\gamma, \alpha_j = a_j/\alpha, \beta_j = b_j/\beta$. The condition for asymptotic stability now simply reads $\gamma \in \mathbb{R}$. Using straightforward calculation, γ can be expressed as $\gamma = \frac{1}{z} \arccos \left(\frac{1}{2} \text{Tr} e^{iz \sum_i g_i \sigma^i} \right)$ and is, interestingly, only a function of the magnitudes α, β and the z-projections α_3 and β_3:

$$\gamma(z) = \frac{1}{z} \arccos Q(z), \tag{11}$$

where

$$Q(z) = \frac{1}{8} \Bigg(\left(1 - \alpha_3^2 + \left(1 + 3\alpha_3^2 \right) \cos(\alpha z) \right) \Bigg(\left(1 + \beta_3^2 \right) \cos(\beta z)$$

$$+ \left(1 - \beta_3^2 \right) \cosh \left(\frac{\beta z}{\sqrt{3}} \right) \Bigg) - 2\alpha_3 (3 + \alpha_3^2) \beta_3 \sin(\alpha z) \sin(\beta z)$$

$$+ 2 \left(1 - \alpha_3^2 \right) \cosh \left(\frac{\alpha z}{2\sqrt{3}} \right) \left(\left(1 + \beta_3^2 \right) \cos \left(\frac{\alpha z}{2} \right) \cos(\beta z) \right.$$

$$+ \left(1 - \beta_3^2 \right) \cos \left(\frac{\alpha z}{2} \right) \cosh \left(\frac{\beta z}{\sqrt{3}} \right) - 2\alpha_3 \beta_3 \sin \left(\frac{\alpha z}{2} \right) \sin(\beta z) \Bigg) \Bigg). \tag{12}$$

Now the stability condition reduces to $|Q(z)| \leqslant 1$. For small steps z, the expression $Q(z)$ in (12) can be written as a power series in z:

$$Q(z) = 1 - \frac{1}{6} \left(\alpha^2 + \beta^2 + 2a_3^2 + 2b_3^2 + 6a_3 b_3 \right) z^2 + \mathcal{O}(z^4). \tag{13}$$

It can easily be proven diagonalizing the quadratic form that the z^2 term is always non-positive; hence, the decomposition scheme is indeed always (for any a_j, b_j) stable, for the small steps z.
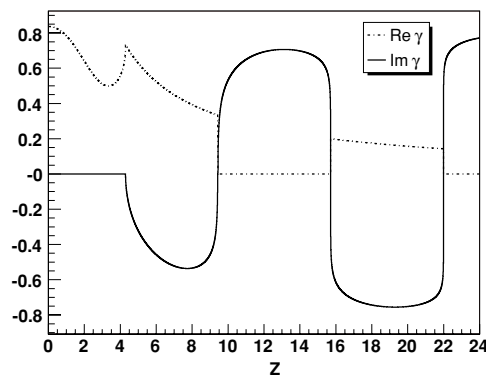
Figure 4. Illustration of the stability threshold for 2×2 case. Since matrices are traceless, collision of eigenvalues of $U(z)$ takes place on the real axis. In the figure we plot Reγ (dashed) and Im γ (full), as a function of z for the case $\alpha = \beta = 1$ and $\alpha_3 = \beta_3 = 0.1$.

Figure 4 illustrates how eigenvalues for the small steps z always lie on the unit circle in the complex plane. When the step z is being increased, the eigenvalues are travelling along the unit circle, one in a clockwise and the other in a counter-clockwise direction. At some point, namely at $z = z_{max}$, a collision occurs and a pair of eigenvalues bounce off the unit circle; then γ becomes complex. However, because of the restriction $|\det U| = 1$ their product remains on the unit circle. Our 2×2 matrices A and B are assumed to be traceless; therefore, collisions always occur on the real axis and the eigenvalues are both real during the bounce.

4. Conclusion

We have proposed a simple explicit complex-coefficient split-step decomposition of an operator exponential, based on Suzuki's scheme, for a sum of arbitrary number of operators. As compared to an optimal scheme with real coefficients, our scheme requires less terms for the same order; furthermore, we can gain an extra order at no additional expense. Despite having complex coefficients, the decomposition is always stable for a sufficiently small step size, and can be stabilized by additional renormalization of the state vector.

We suggest that our method may be used in conjunction with other methods for efficient time evolution of complex quantum systems (one application has already been done in [10]), or interacting many-body quantum systems, such as for example, with time-dependent DMRG methods [11–13] where efficient and accurate estimation of operator exponentials for short time steps is one of the cruicial black-box operations.

On the other hand, the proposed method may also challenge the efficiency of high-order split-step symplectic integration methods (e.g. [14]) for solving classical Hamilton equations. Our method provides smaller and higher remainders for a smaller number of decomposition factors at the cost of complex arithmetics. It would be particularly interesting to compare our approach to (or perhaps even combine with) the recent optimized approach to symplectic integration using higher order *sub-propagators* [15].

Acknowledgments

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