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Multi-Product Expansion with Suzuki's Method: Generalization

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Abstract. In this paper we discuss the extension to exponential splitting methods with respect to time-dependent operators. We concentrate on the Suzuki's method, which incorporates ideas to the time-ordered exponential of [3, 11, 12, 34]. We formulate the methods with respect to higher order by using kernels for an extrapolation scheme. The advantages include more accurate and less computational intensive schemes to special time-dependent harmonic oscillator problems. The benefits of the higher order kernels are given on different numerical examples.

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Key words: Suzuki's method, multiproduct expansion, multiplicate and additive splitting schemes, exponential splitting.

1. Introduction

In this paper we concentrate on approximation to the solution of the linear evolution equation, e.g., time-dependent Schrödinger equation,

$$\partial_t u = L(t)u = (A(t) + B(t))u, \qquad u(0) = u_0, \tag{1.1}$$

where L,A and B are unbounded and time-dependent operators. For such equations, we concentrate on comparing the higher order methods to Suzuki's schemes. Here the Suzuki's methods apply factorized symplectic algorithms with forward derivatives, see, e.g., [11, 12]. Some preliminary comparison are presented in [3, 11], where the benefits of each method are outlined.

In our paper, we like to see the drawback of each method, so for the Magnus integrator, the spiked harmonic oscillator case, see [12] and for the Suzuki‘s method, geometric properties, which are known to be solved with geometric integrator, e.g. Magnus integrators.

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At least we like to outline an idea to combine the Magnus integrators and the Suzuki‘s factorization schemes to optimize the methods.

The paper is outlined as follows. In Section 2, we present our Suzuki's rule for decomposing time-ordered integrators. The extrapolation schemes and their generalization are given in Section 3. In Section 4, we present the error analysis of the multi-product splitting based on the extrapolation analysis. The numerical experiments are given in Section 5, here time-dependent problems are discussed. In Section 6, we briefly summarize our results.

2. Exponential splitting method based on Suzuki's time-ordered exponential

Instead of the Magnus expansion, see [10], one can also directly implement the time-ordered exponential as suggested by Suzuki [34]. We deal with a linear evolution equation given as:

$$\frac{dY}{dt} = A(t)Y(t), \tag{2.1}$$

with solution

$$Y(t) = \exp(\Omega(t))Y(0). \tag{2.2}$$

This can be expressed as:

$$Y(t) = \mathscr{T}\left(\exp(\int_0^t A(s)\, ds\right) Y(0)\,, \tag{2.3}$$

where the time-ordering operator $\mathscr{T}$ is given in [15]. Rewriting (2.3) as

$$Y(t+\Delta t) = \mathscr{T}\left(\exp\int_t^{t+\Delta t} A(s)ds\right)Y(t). \tag{2.4}$$

Aside from the conventional expansion

$$\begin{aligned}&\mathscr{T}\left(\exp\int_t^{t+\Delta t} A(s)ds\right)\\ =&1+\int_t^{t+\Delta t} A(s_1)ds_1+\int_t^{t+\Delta t} ds_1\int_t^{s_1} ds_2 A(s_1)A(s_2)+\cdots\,,\end{aligned} \tag{2.5}$$

the time-ordered exponential can also be interpreted more intuitively as

$$\mathscr{T}\left(\exp\int_t^{t+\Delta t} A(s)ds\right) = \lim_{n\to\infty}\mathscr{T}\left(\mathrm{e}^{\frac{\Delta t}{n}\sum_{i=1}^n A\left(t+i\frac{\Delta t}{n}\right)}\right), \tag{2.6}$$

$$= \lim_{n\to\infty}\mathrm{e}^{\frac{\Delta t}{n}A(t+\Delta t)}\cdots\mathrm{e}^{\frac{\Delta t}{n}A\left(t+\frac{2\Delta t}{n}\right)}\mathrm{e}^{\frac{\Delta t}{n}A\left(t+\frac{\Delta t}{n}\right)}. \tag{2.7}$$